LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
Data File : BM028551.D
Acq On : 26 Jan 2021 21:22
Operator : CG/JU
Sample : M1217-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1617

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM028551.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.569	62	65	78	rBV	19063	28547	1.27%	0.074%
2	5.516	389	396	403	rBV	586489	838187	37.36%	2.180%
3	6.645	582	588	593	rVB	18668	28724	1.28%	0.075%
4	7.151	666	674	688	rVB	539107	882653	39.34%	2.296%
5	7.592	742	749	754	rBV2	108401	191204	8.52%	0.497%
6	7.769	772	779	791	rBV	13560	27108	1.21%	0.071%
7	7.987	806	816	823	rBV	135650	221809	9.89%	0.577%
8	8.122	832	839	844	rVB	82547	124491	5.55%	0.324%
9	8.204	848	853	861	rVB2	36776	54886	2.45%	0.143%
10	8.634	921	926	938	rVB5	13691	33245	1.48%	0.086%
11	9.116	995	1008	1011	rBV2	51959	101770	4.54%	0.265%
12	9.163	1011	1016	1021	rVV	347707	570995	25.45%	1.485%
13	9.216	1021	1025	1030	rVB	60087	87801	3.91%	0.228%
14	10.204	1188	1193	1199	rBV4	18268	38978	1.74%	0.101%
15	10.763	1282	1288	1291	rBV	125106	197675	8.81%	0.514%
16	10.804	1291	1295	1301	rVB	174901	274337	12.23%	0.714%
17	10.975	1316	1324	1329	rVB	101977	156447	6.97%	0.407%
18	11.704	1442	1448	1454	rBV4	20852	39945	1.78%	0.104%
19	11.857	1469	1474	1479	rVB3	30020	46511	2.07%	0.121%
20	11.986	1487	1496	1502	rBV4	24774	58042	2.59%	0.151%
21	12.169	1521	1527	1530	rBV	124806	185794	8.28%	0.483%
22	12.222	1530	1536	1545	rVB2	85190	205860	9.18%	0.535%
23	12.339	1551	1556	1564	rVB3	84026	131772	5.87%	0.343%
24	12.451	1567	1575	1578	rVV3	77890	158584	7.07%	0.412%
25	12.480	1578	1580	1585	rVB	87767	110240	4.91%	0.287%
26	12.580	1593	1597	1607	rBV5	15262	50780	2.26%	0.132%
27	12.710	1616	1619	1624	rVB3	20725	29516	1.32%	0.077%
28	12.839	1636	1641	1645	rBV3	25910	40555	1.81%	0.105%
29	12.898	1645	1651	1655	rBV7	14306	34782	1.55%	0.090%
30	13.016	1668	1671	1676	rVB	38634	50141	2.23%	0.130%
31	13.157	1693	1695	1702	rVB2	28455	36561	1.63%	0.095%
32	13.257	1702	1712	1720	rBV	767895	1147890	51.16%	2.986%
33	13.333	1722	1725	1732	rVV5	16232	36947	1.65%	0.096%
34	13.445	1740	1744	1750	rVB	131556	177464	7.91%	0.462%
35	13.521	1752	1757	1763	rBV	296372	481034	21.44%	1.251%
36	14.057	1843	1848	1849	rBV2	59027	80164	3.57%	0.209%

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
Data File : BM028551.D
Acq On : 26 Jan 2021 21:22
Operator : CG/JU
Sample : M1217-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1617

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.086	1850	1853	1859	rVV2	91635	173256	7.72%	0.451%
38	14.151	1860	1864	1868	rVB3	69785	104538	4.66%	0.272%
39	14.221	1873	1876	1879	rVB	43701	47340	2.11%	0.123%
40	14.257	1879	1882	1884	rBV	24102	29694	1.32%	0.077%
41	14.374	1899	1902	1903	rBV3	26250	27797	1.24%	0.072%
42	14.404	1903	1907	1911	rVB	179427	227601	10.14%	0.592%
43	14.457	1912	1916	1921	rVB3	76499	123977	5.53%	0.322%
44	14.516	1922	1926	1934	rBV	109889	166586	7.43%	0.433%
45	14.598	1936	1940	1941	rBV3	36620	50468	2.25%	0.131%
46	14.633	1942	1946	1950	rVV2	248932	425240	18.95%	1.106%
47	14.692	1953	1956	1962	rVB	200123	264565	11.79%	0.688%
48	14.786	1968	1972	1976	rVB	141553	182559	8.14%	0.475%
49	14.851	1976	1983	1993	rVB	542011	906597	40.41%	2.358%
50	14.957	1996	2001	2006	rBV	207702	306795	13.67%	0.798%
51	15.051	2013	2017	2024	rVB2	106816	170890	7.62%	0.444%
52	15.133	2028	2031	2037	rVB4	41781	80315	3.58%	0.209%
53	15.245	2046	2050	2053	rBV	85820	116621	5.20%	0.303%
54	15.410	2075	2078	2082	rBV2	52824	71000	3.16%	0.185%
55	15.463	2083	2087	2091	rVB	96310	115502	5.15%	0.300%
56	15.733	2129	2133	2145	rVB	156307	268916	11.99%	0.699%
57	15.962	2169	2172	2178	rVB	51566	73937	3.30%	0.192%
58	16.115	2193	2198	2204	rVB	544597	744882	33.20%	1.937%
59	16.333	2229	2235	2240	rBV	393771	609562	27.17%	1.585%
60	16.474	2257	2259	2264	rVB2	69784	89082	3.97%	0.232%
61	16.574	2272	2276	2283	rVB	344569	429716	19.15%	1.118%
62	16.651	2284	2289	2291	rBV	135684	209875	9.35%	0.546%
63	16.680	2291	2294	2298	rVV	793613	1058736	47.19%	2.754%
64	16.715	2298	2300	2304	rVB	164505	174539	7.78%	0.454%
65	16.768	2305	2309	2310	rBV	100371	118467	5.28%	0.308%
66	16.798	2310	2314	2320	rVB	275106	413782	18.44%	1.076%
67	16.862	2321	2325	2329	rBV	150022	223098	9.94%	0.580%
68	16.957	2337	2341	2345	rVB	133707	175646	7.83%	0.457%
69	17.015	2348	2351	2353	rVV	72996	97085	4.33%	0.253%
70	17.039	2353	2355	2360	rVB	138465	159060	7.09%	0.414%
71	17.104	2364	2366	2370	rVB	63957	70424	3.14%	0.183%
72	17.157	2372	2375	2379	rVB	108224	146780	6.54%	0.382%
73	17.362	2406	2410	2415	rBV	243149	330477	14.73%	0.860%
74	17.939	2504	2508	2513	rVB	369732	506994	22.60%	1.319%
75	18.015	2518	2521	2530	rVB2	273213	395956	17.65%	1.030%
76	18.156	2542	2545	2549	rBV	235187	256780	11.45%	0.668%

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Instrument : BNA_M
ClientSampleId : 1617

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
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Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
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77	18.239	2554	2559	2568	rVB3	1195853	2243538	100.00%	5.835%
78	18.527	2605	2608	2616	rVB3	195486	353164	15.74%	0.919%
79	19.092	2700	2704	2710	rBV2	611877	856457	38.17%	2.228%
80	19.309	2738	2741	2746	rBV	308164	403910	18.00%	1.051%
81	19.515	2770	2776	2778	rBV3	553872	1079911	48.13%	2.809%
82	19.551	2778	2782	2790	rVB	1034091	1551599	69.16%	4.036%
83	19.962	2848	2852	2856	rVB	1008711	1238871	55.22%	3.222%
84	20.439	2930	2933	2942	rVB2	476214	731489	32.60%	1.903%
85	20.603	2959	2961	2964	rVB	244871	212400	9.47%	0.552%
86	20.639	2964	2967	2971	rBV	1037844	1184576	52.80%	3.081%
87	21.409	3095	3098	3101	rVB2	384467	427992	19.08%	1.113%
88	21.503	3111	3114	3119	rVB2	241069	284649	12.69%	0.740%
89	21.556	3121	3123	3124	rBV	196575	162370	7.24%	0.422%
90	21.586	3124	3128	3131	rVB	1043564	1177276	52.47%	3.062%
91	22.339	3252	3256	3260	rBV	376652	489109	21.80%	1.272%
92	22.527	3282	3288	3293	rBV	1084832	1831920	81.65%	4.765%
93	22.568	3293	3295	3300	rVB	222980	265314	11.83%	0.690%
94	23.433	3438	3442	3448	rVB	261587	409411	18.25%	1.065%
95	23.674	3476	3483	3489	rBV	891414	1784704	79.55%	4.642%
96	23.727	3489	3492	3496	rVV	168065	280996	12.52%	0.731%
97	23.774	3497	3500	3506	rVB2	180170	306056	13.64%	0.796%
98	24.850	3678	3683	3692	rVB	197678	426054	18.99%	1.108%
99	25.174	3730	3738	3746	rBV	715597	1777652	79.23%	4.624%
100	27.244	4079	4090	4102	rBV	530303	1860764	82.94%	4.840%

Sum of corrected areas: 38446756

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
Data File : BM028551.D
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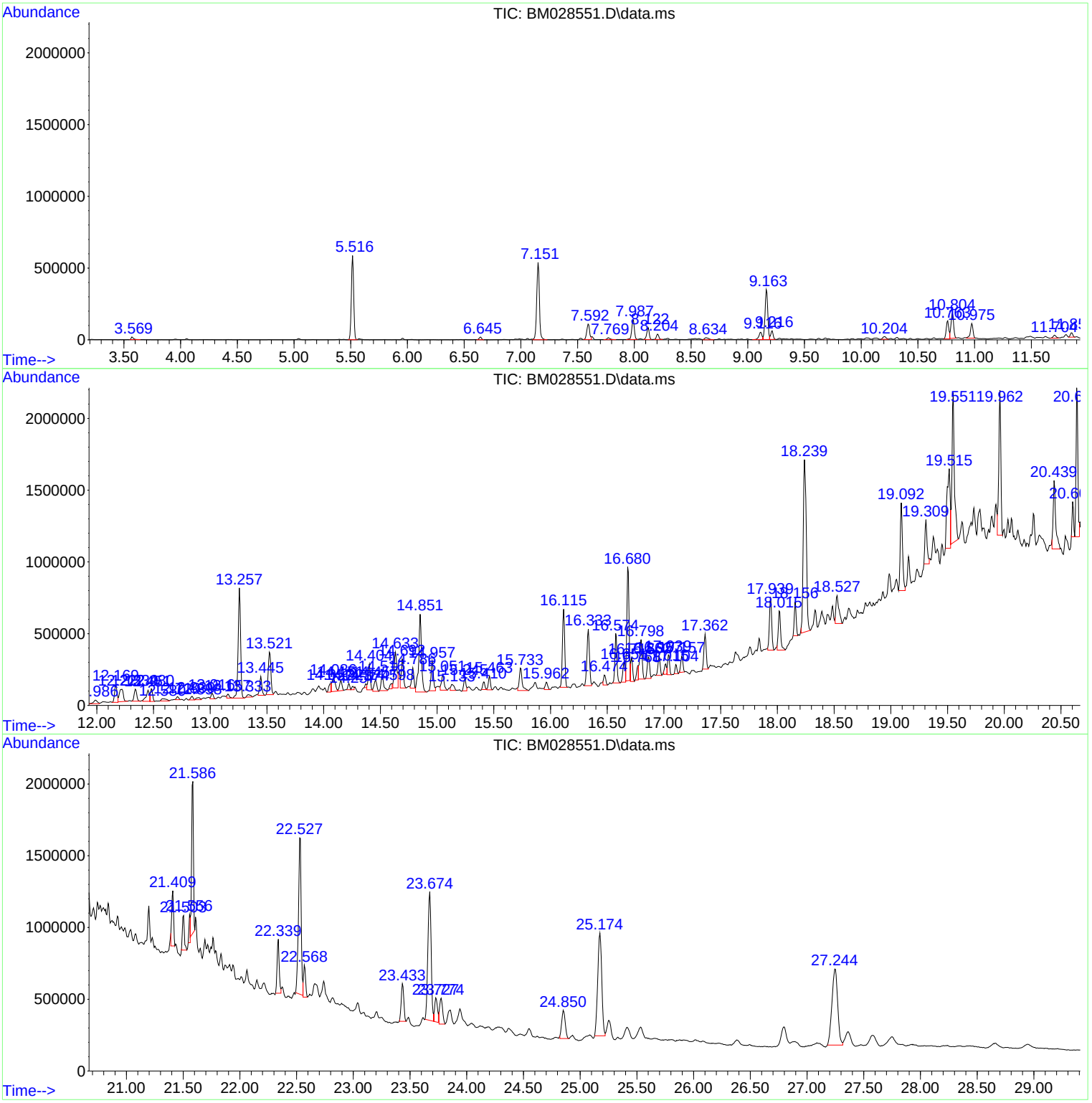
Sample : M1217-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
1617

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
Data File : BM028551.D
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Operator : CG/JU
Sample : M1217-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1617

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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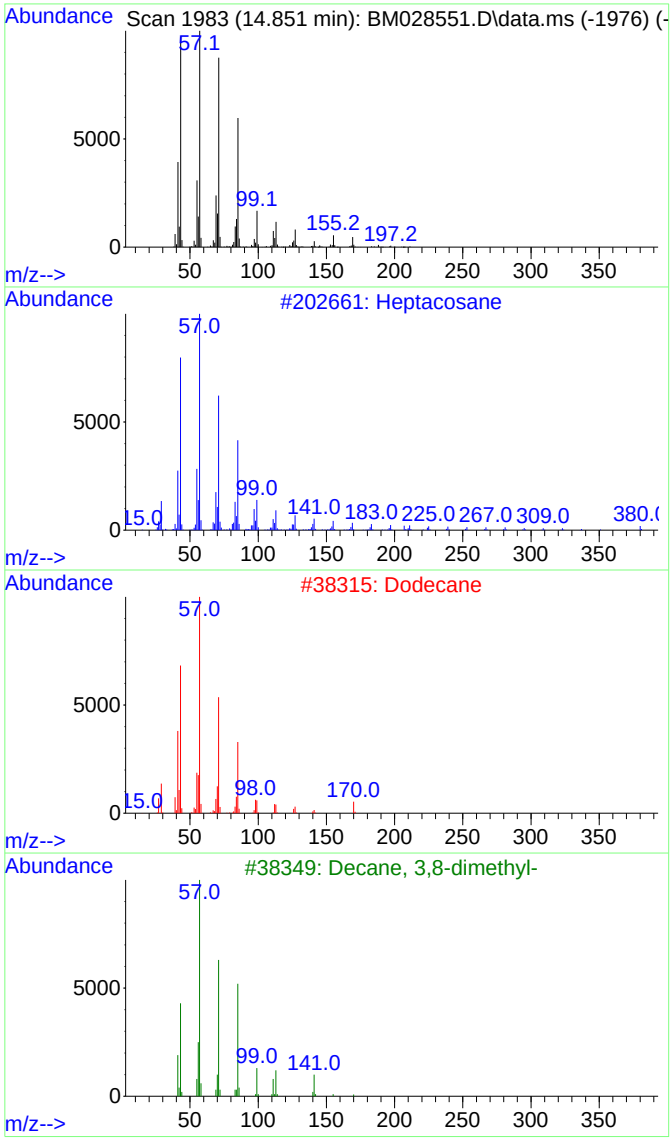
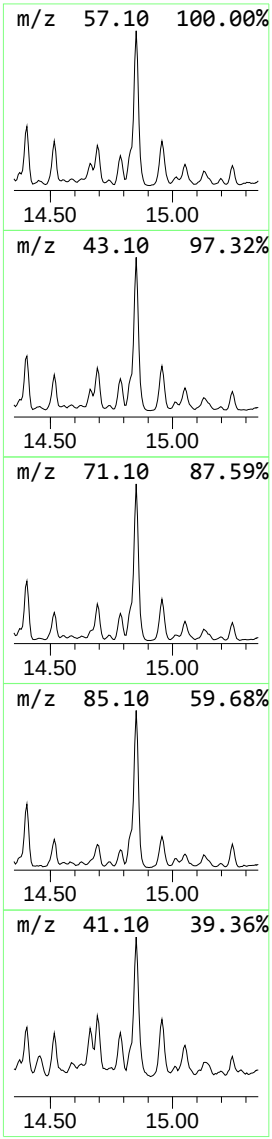
Peak Number 1 Heptacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.851	42.64 ng	906597	Acenaphthene-d10	14.633

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Dodecane	170	C12H26	000112-40-3	90
3	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
4	Hexacosane	366	C26H54	000630-01-3	86
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
Data File : BM028551.D
Acq On : 26 Jan 2021 21:22
Operator : CG/JU
Sample : M1217-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1617

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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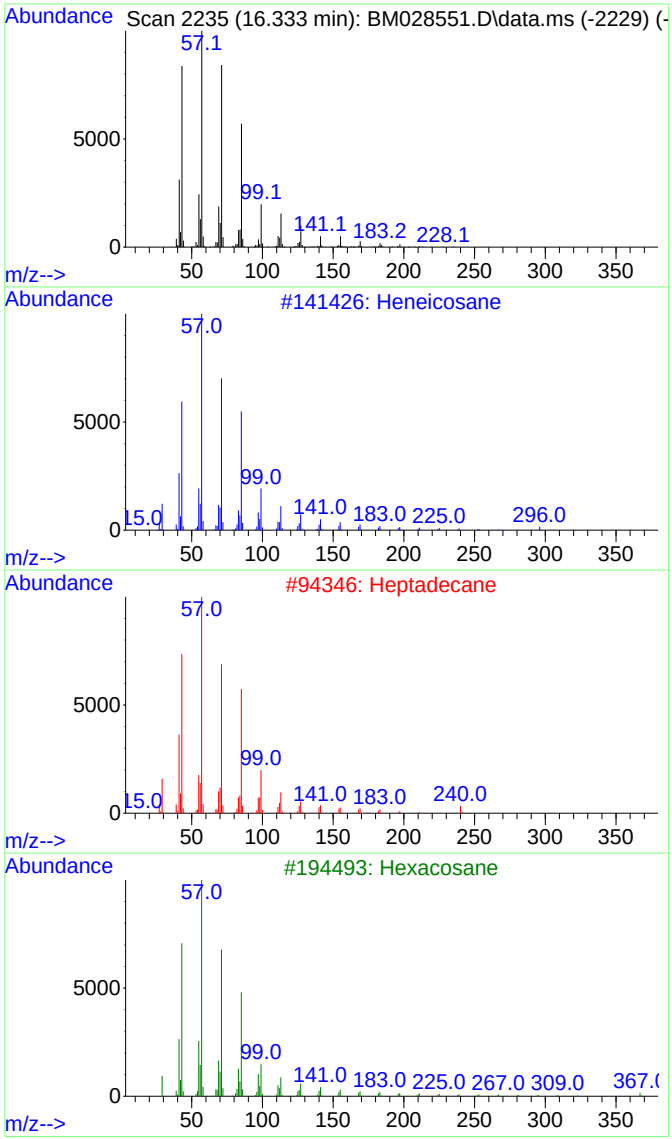
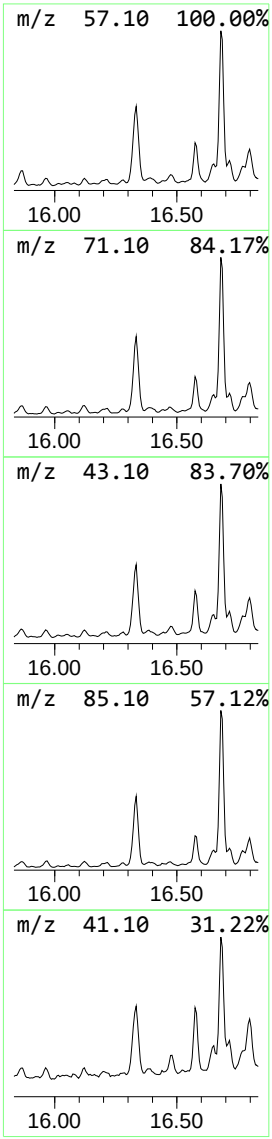
Peak Number 2 Heneicosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.333	36.89 ng	609562	Phenanthrene-d10	17.362

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane	240	C17H36	000629-78-7	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	Heptacosane	380	C27H56	000593-49-7	87
5	Octacosane	394	C28H58	000630-02-4	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
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Instrument : BNA_M
ClientSampleId : 1617

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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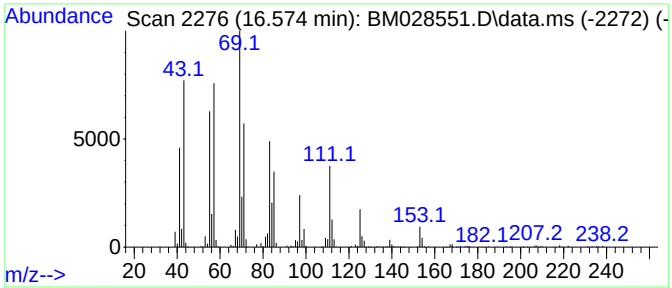
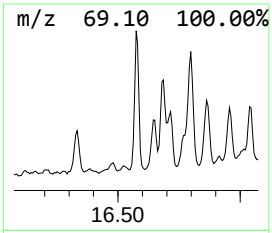
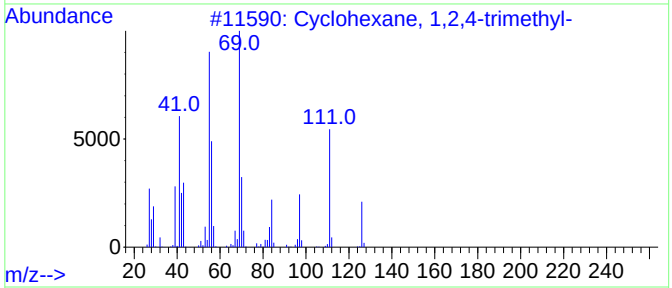
Peak Number 3 Cyclohexane, 1,2,4-trimethyl- Concentration Rank 19

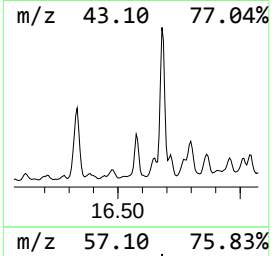
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.574	26.01 ng	429716	Phenanthrene-d10	17.362

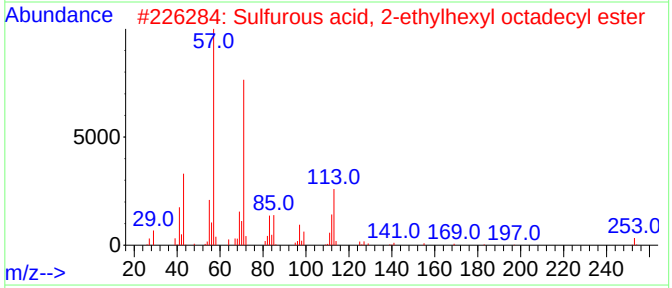
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	55
2	Sulfurous acid, 2-ethylhexyl oct...	446	C26H54O3S	1000309-20-1	22
3	Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	22
4	2,3-Dimethyl-3-heptene, (Z)-	126	C9H18	059643-73-1	18
5	Nonane, 4,5-dimethyl-	156	C11H24	017302-23-7	18

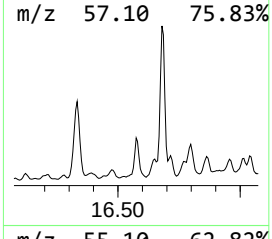


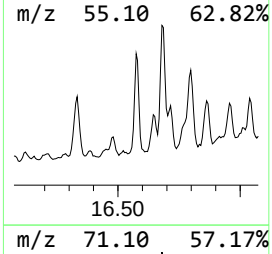


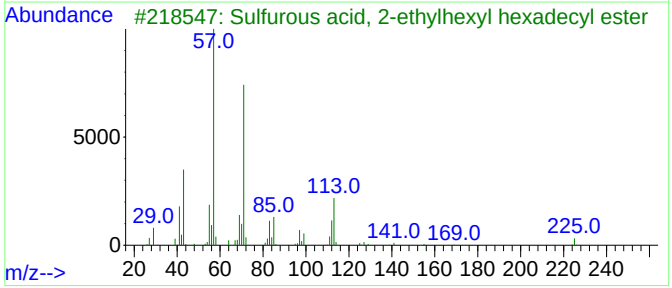


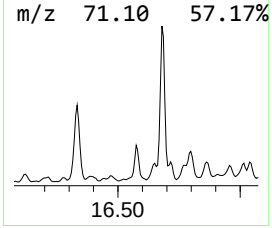












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Data File : BM028551.D
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Instrument : BNA_M
ClientSampleId : 1617

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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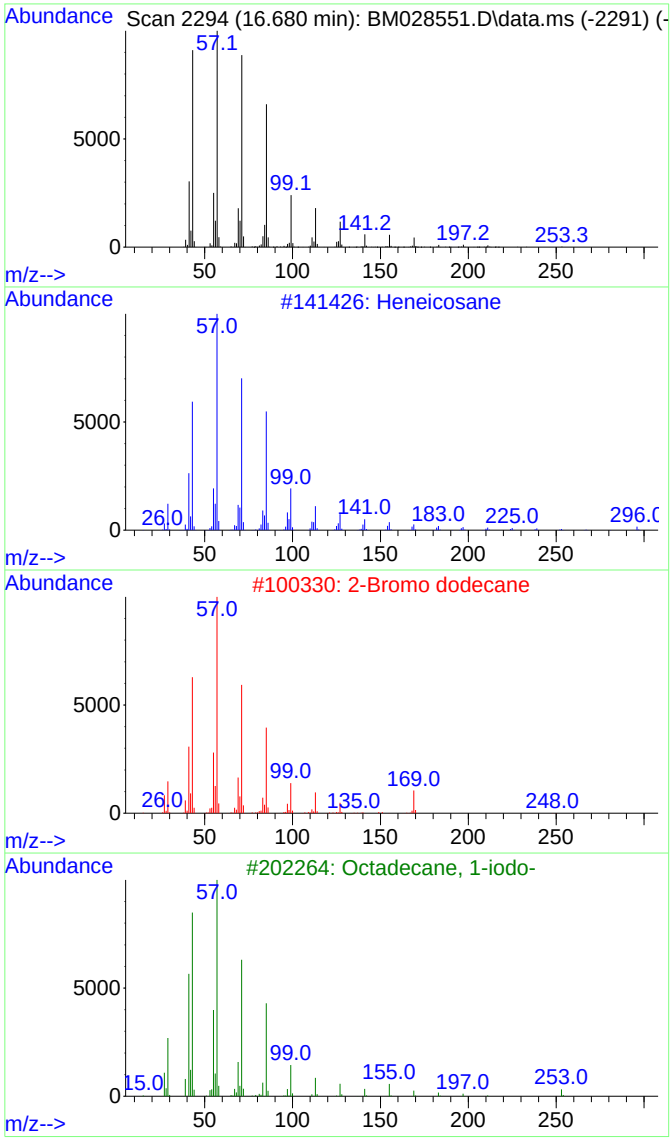
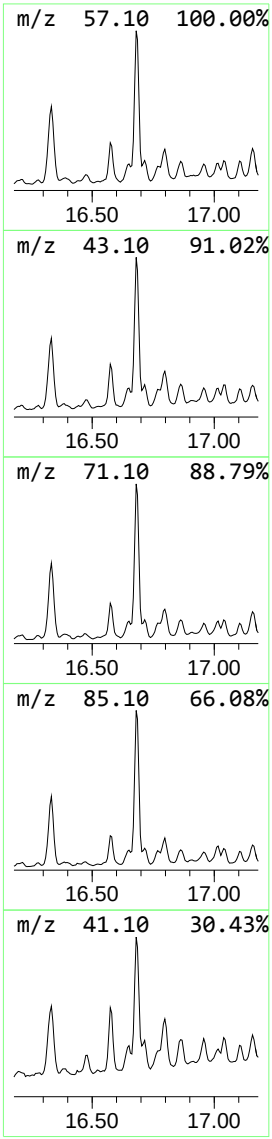
Peak Number 4 2-Bromo dodecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.680	64.07 ng	1058740	Phenanthrene-d10	17.362

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	2-Bromo dodecane	248	C12H25Br	013187-99-0	90
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
4	Heptadecane	240	C17H36	000629-78-7	86
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	64





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Data File : BM028551.D
Acq On : 26 Jan 2021 21:22
Operator : CG/JU
Sample : M1217-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1617

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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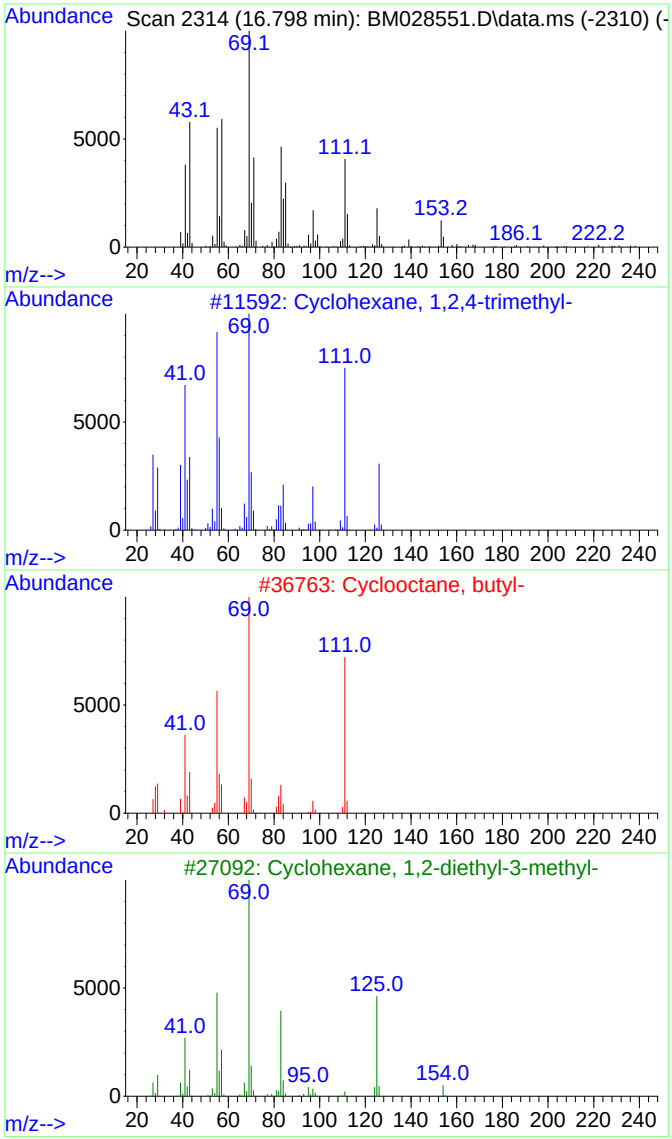
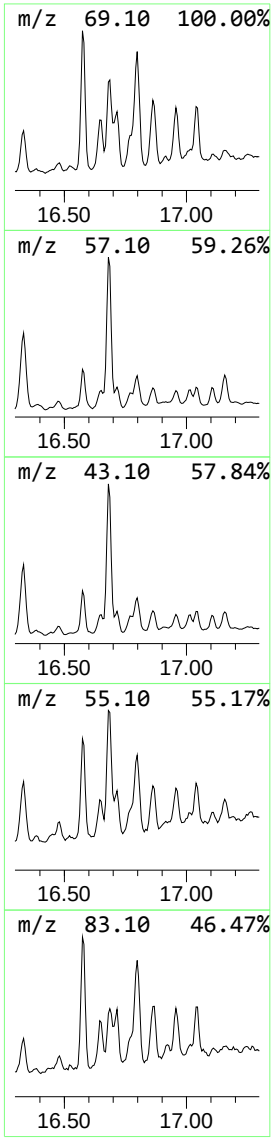
Peak Number 5 unknown16.798 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.798	25.04 ng	413782	Phenanthrene-d10	17.362

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	49
2	Cyclooctane, butyl-	168	C12H24	016538-93-5	38
3	Cyclohexane, 1,2-diethyl-3-methyl-	154	C11H22	061141-80-8	38
4	Cyclooctane, (1-methylpropyl)-	168	C12H24	016538-89-9	35
5	3-Isopropyl-5-methyl-hex-4-en-2-one	154	C10H18O	077142-85-9	22





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Sample : M1217-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1617

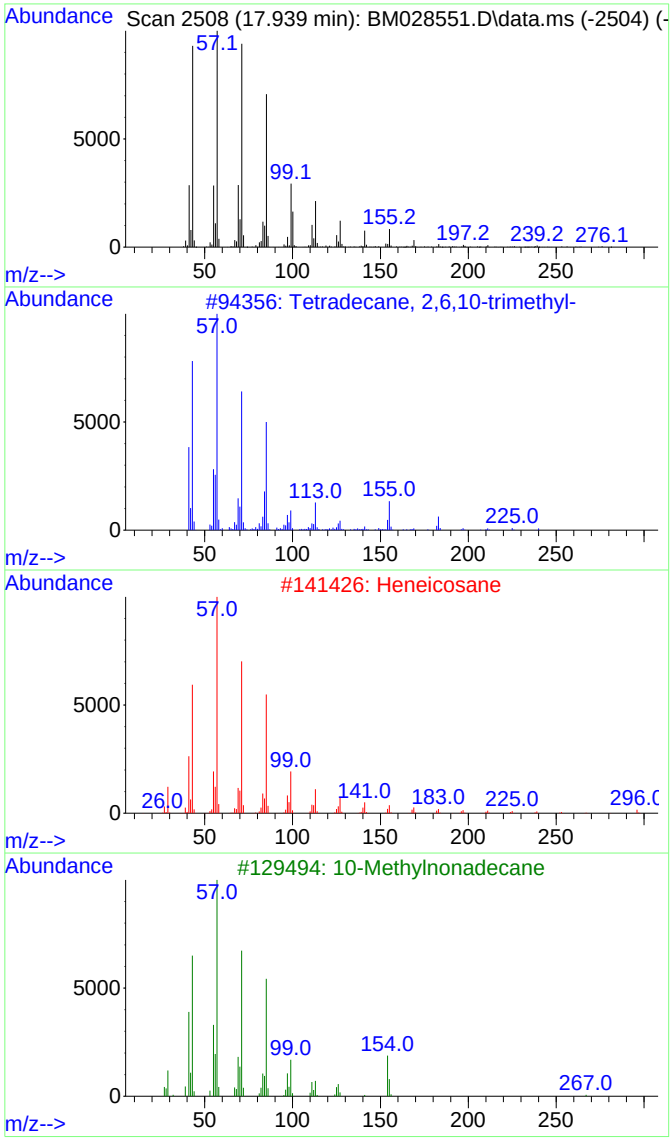
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

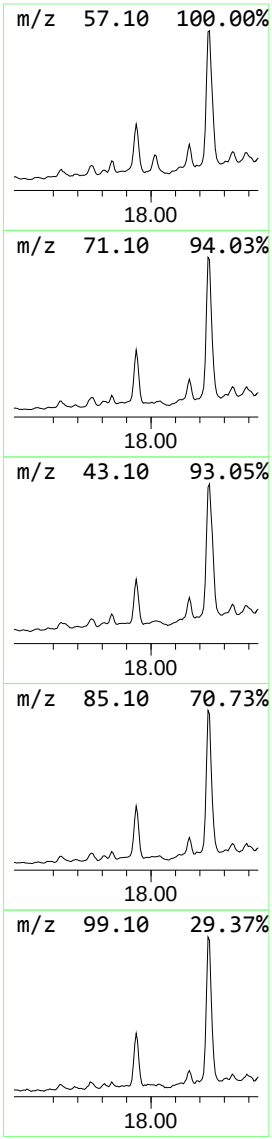
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Tetradecane, 2,6,10-trimethyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.939	30.68 ng	506994	Phenanthrene-d10	17.362

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	72
2	Heneicosane	296	C21H44	000629-94-7	64
3	10-Methylnonadecane	282	C20H42	056862-62-5	64
4	Tridecane, 6-propyl-	226	C16H34	055045-10-8	64
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64





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Sample : M1217-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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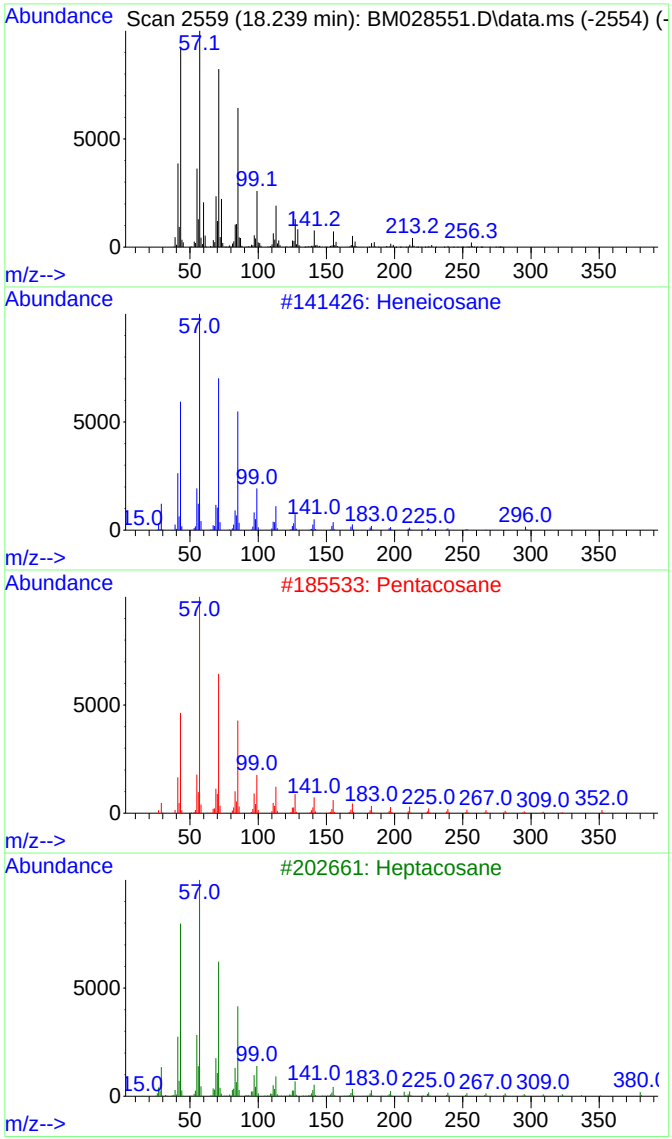
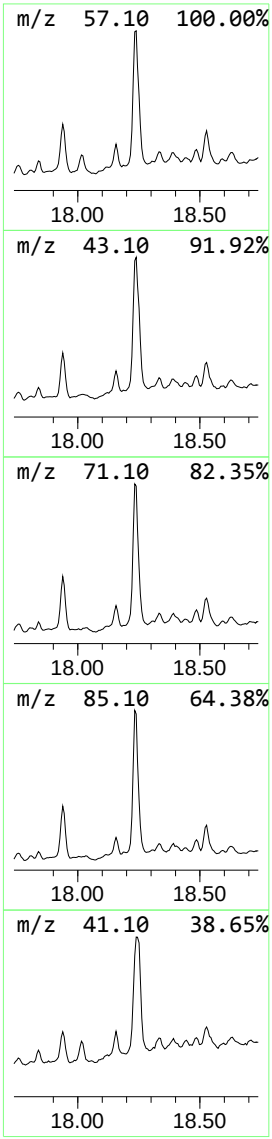
Peak Number 7 Pentacosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.239	135.78 ng	2243540	Phenanthrene-d10	17.362

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	68
2	Pentacosane	352	C25H52	000629-99-2	58
3	Heptacosane	380	C27H56	000593-49-7	58
4	Hexacosane	366	C26H54	000630-01-3	58
5	Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	58





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Operator : CG/JU
Sample : M1217-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1617

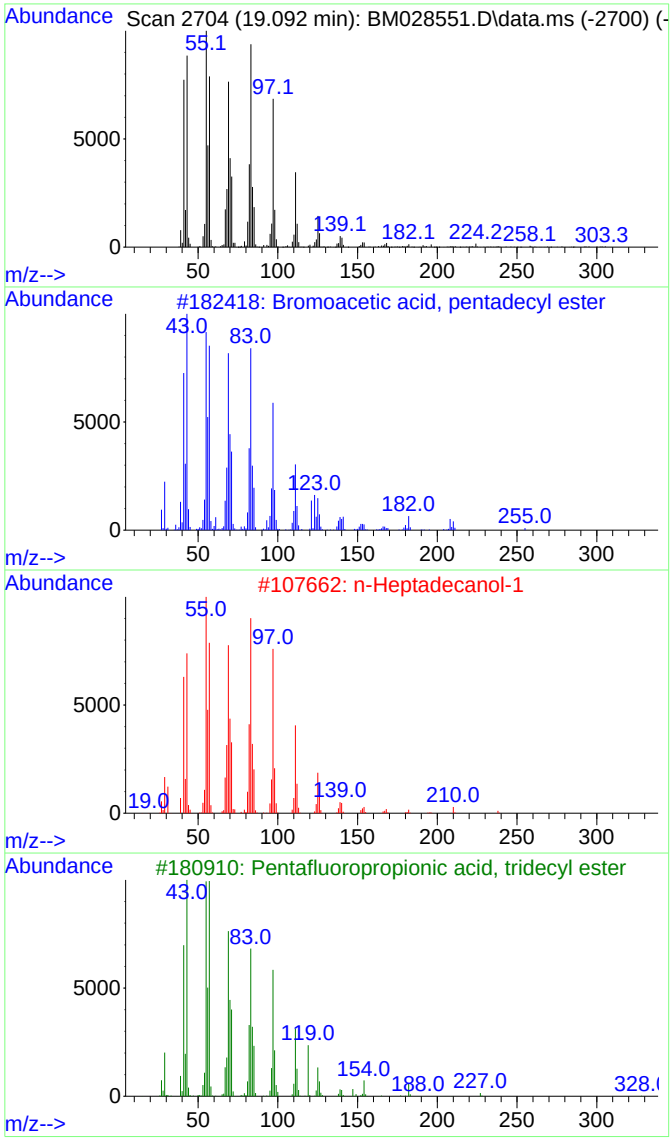
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

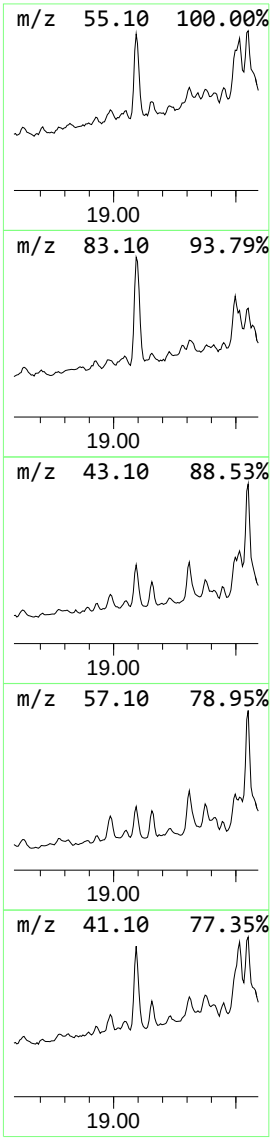
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Bromoacetic acid, pentadecy... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.092	51.83 ng	856457	Phenanthrene-d10	17.362

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	94
2	n-Heptadecanol-1	256	C17H36O	001454-85-9	94
3	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	93
4	n-Pentadecanol	228	C15H32O	000629-76-5	91
5	1-Hexadecanol	242	C16H34O	036653-82-4	91





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Acq On : 26 Jan 2021 21:22
Operator : CG/JU
Sample : M1217-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1617

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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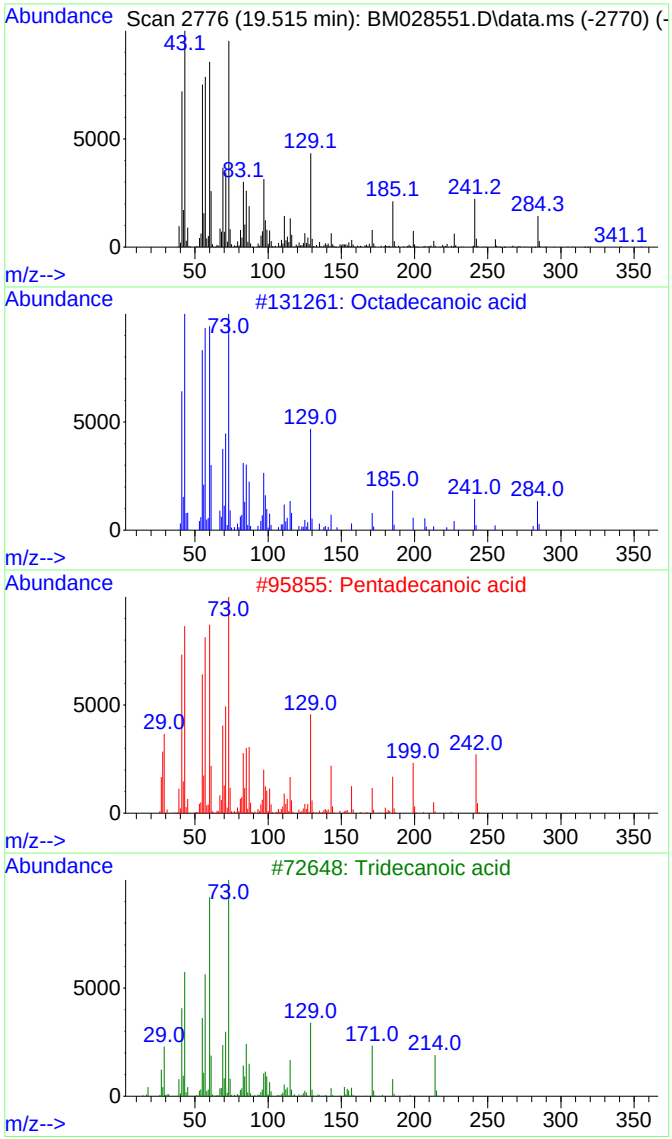
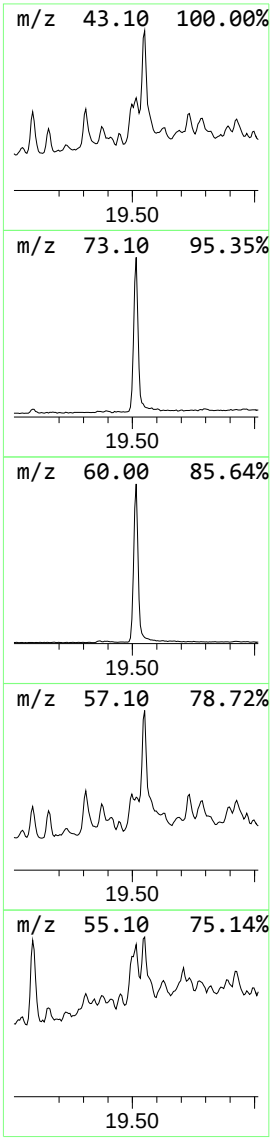
Peak Number 9 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.515	75.88 ng	1079910	Chrysene-d12	21.503

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	70
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68





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Instrument : BNA_M
ClientSampleId : 1617

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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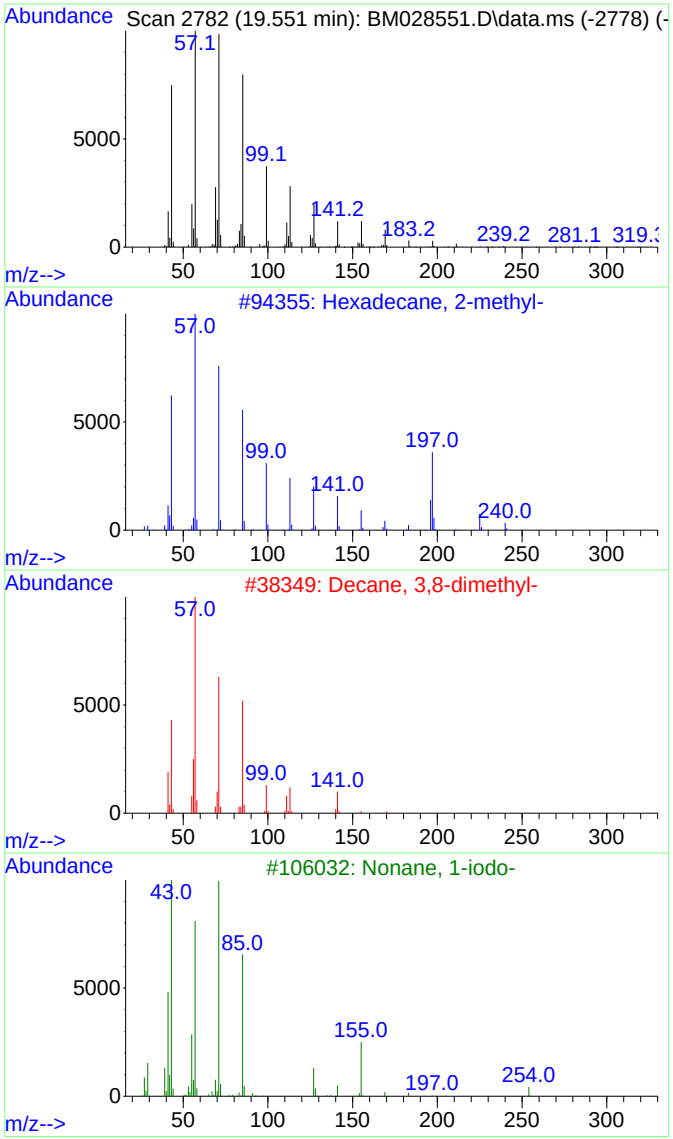
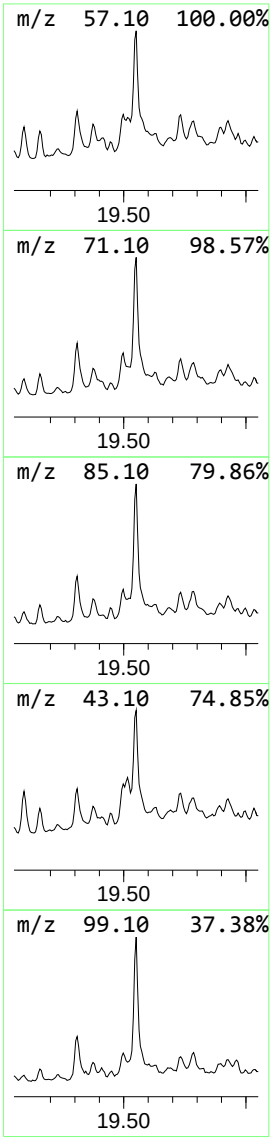
Peak Number 10 Hexadecane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.551	109.02 ng	1551600	Chrysene-d12	21.503

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	64
2	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	58
3	Nonane, 1-iodo-	254	C9H19I	004282-42-2	53
4	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	50
5	Undecane, 5-methyl-	170	C12H26	001632-70-8	50





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Sample : M1217-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1617

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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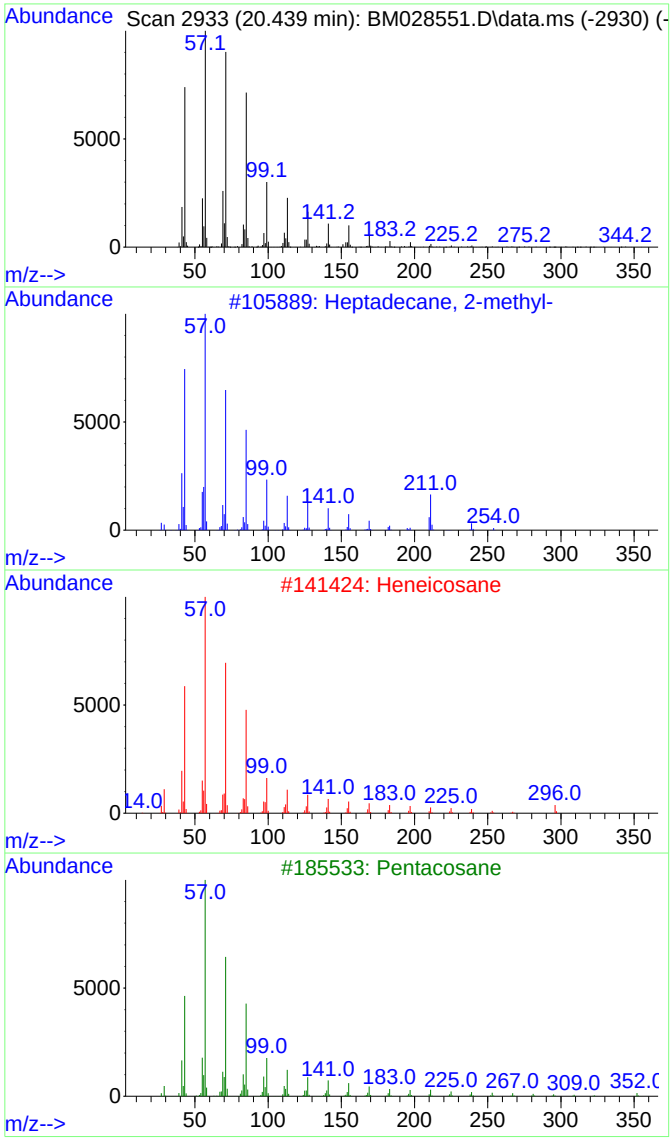
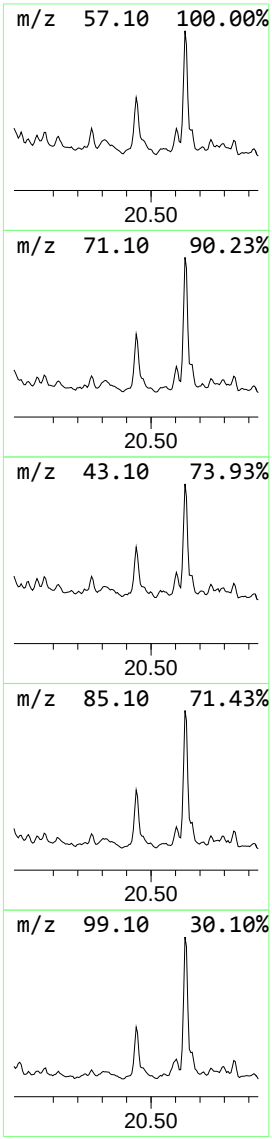
Peak Number 11 Heptadecane, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.439	51.40 ng	731489	Chrysene-d12	21.503

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	83
2	Heneicosane	296	C21H44	000629-94-7	78
3	Pentacosane	352	C25H52	000629-99-2	78
4	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	72
5	Nonane, 5-butyl-	184	C13H28	017312-63-9	64





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Sample : M1217-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1617

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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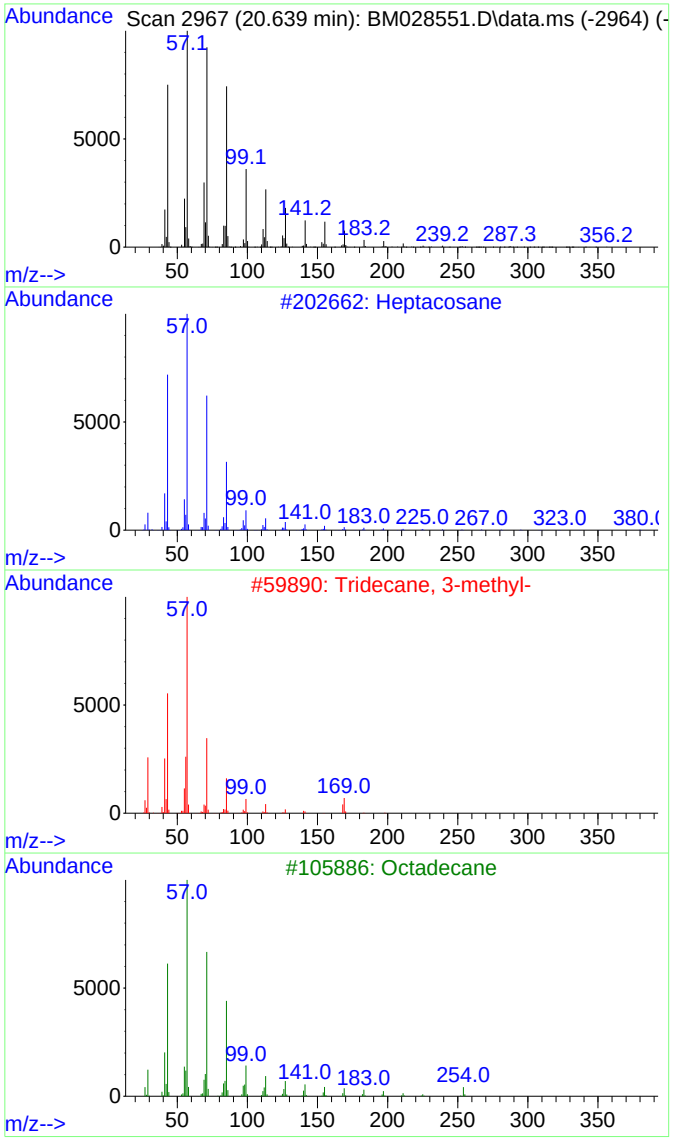
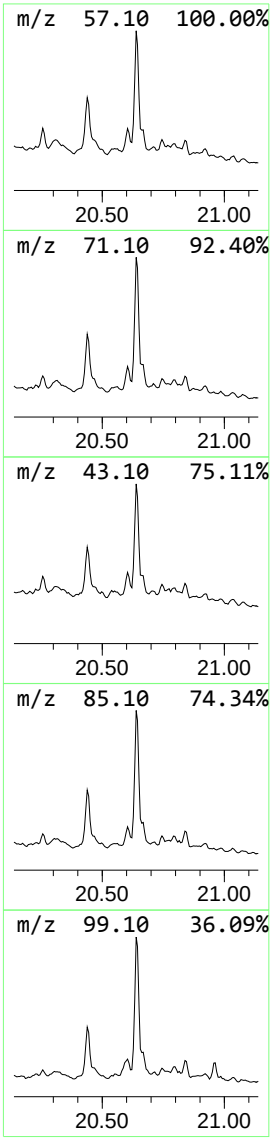
Peak Number 12 Tridecane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.639	83.23 ng	1184580	Chrysene-d12	21.503

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Tridecane, 3-methyl-	198	C14H30	006418-41-3	86
3	Octadecane	254	C18H38	000593-45-3	83
4	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	74
5	Heptadecane	240	C17H36	000629-78-7	72





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Sample : M1217-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1617

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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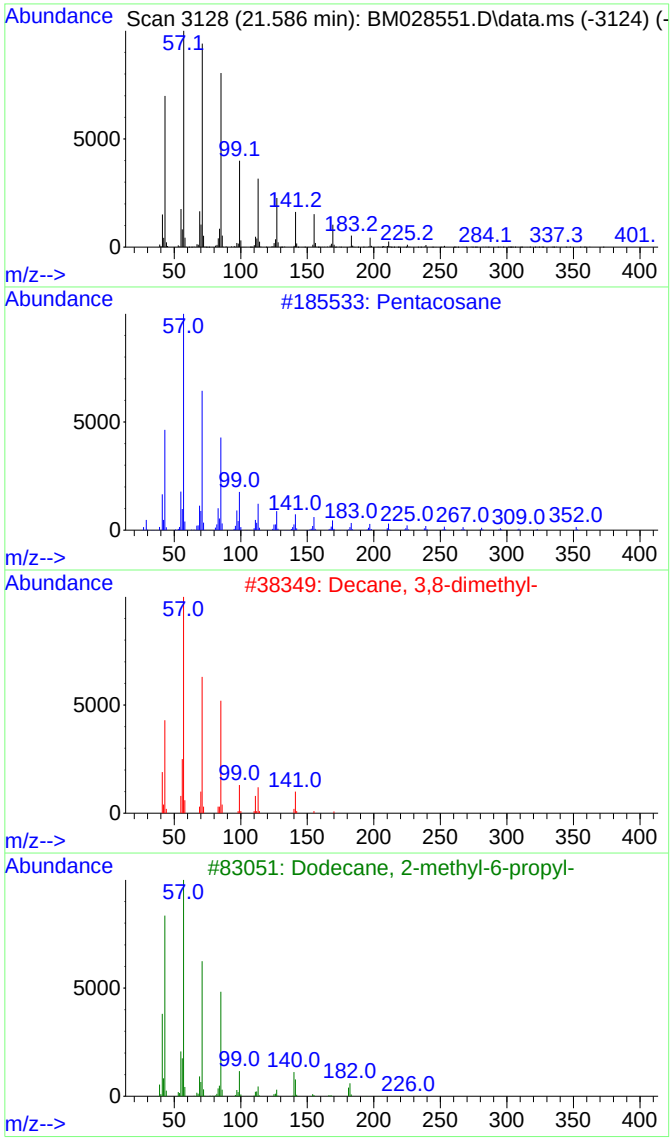
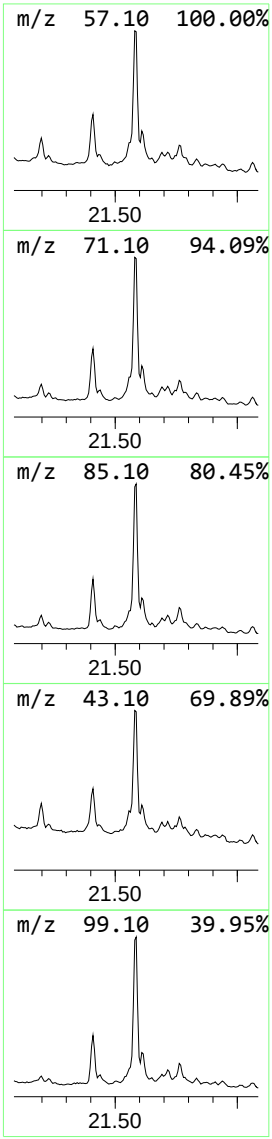
Peak Number 13 Decane, 3,8-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.586	82.72 ng	1177280	Chrysene-d12	21.503

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	90
2	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	58
3	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	52
4	Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	50
5	Dodecane, 4-methyl-	184	C13H28	006117-97-1	46





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ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1617

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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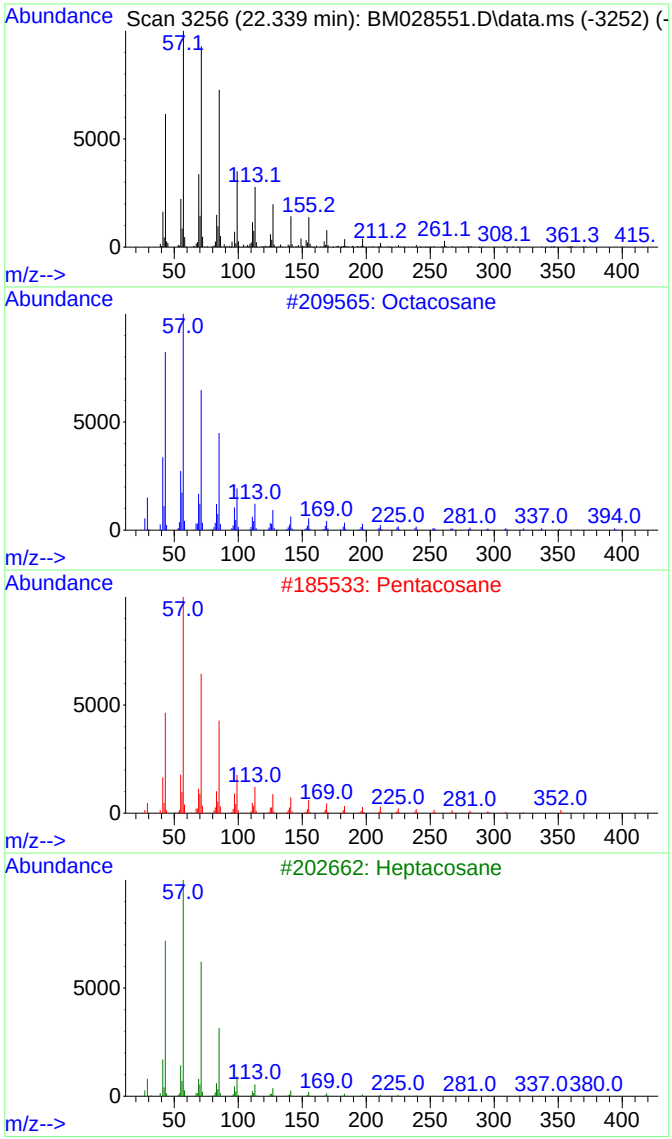
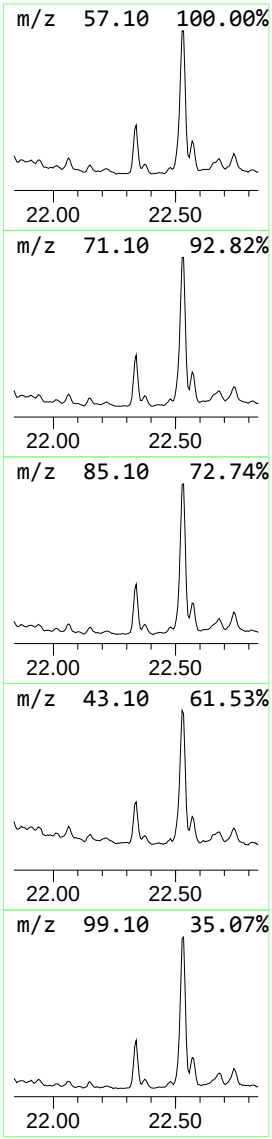
Peak Number 14 Octacosane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.339	34.37 ng	489109	Chrysene-d12	21.503

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Pentacosane	352	C25H52	000629-99-2	90
3	Heptacosane	380	C27H56	000593-49-7	90
4	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	86
5	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	76





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Instrument : BNA_M
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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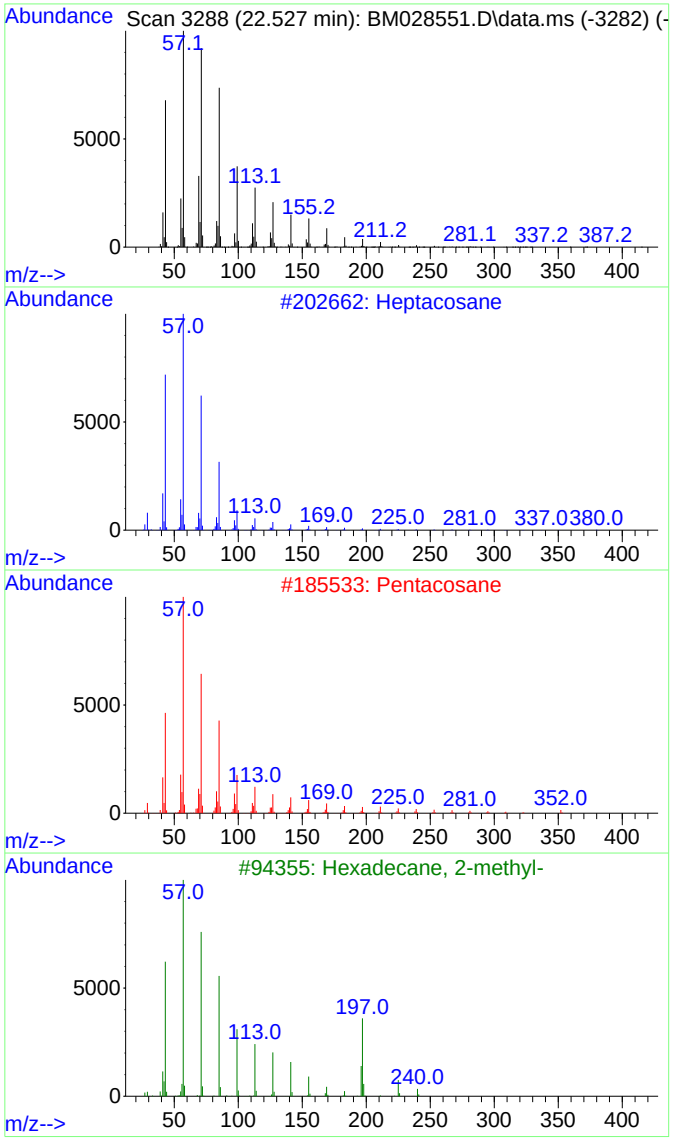
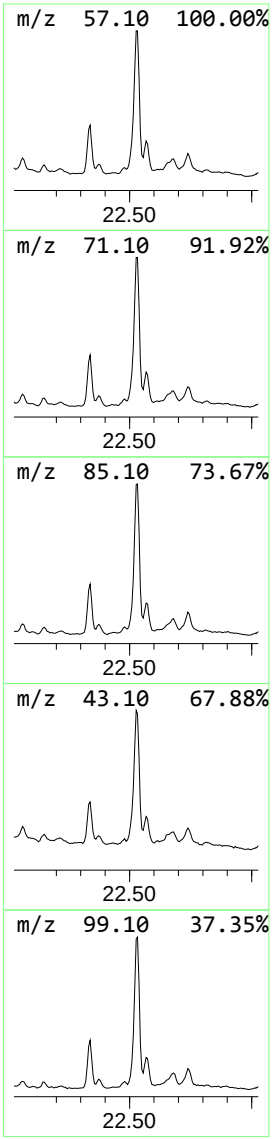
Peak Number 15 unknown22.527 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.527	128.71 ng	1831920	Chrysene-d12	21.503

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Pentacosane	352	C25H52	000629-99-2	90
3	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	78
4	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	78
5	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	74





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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1617

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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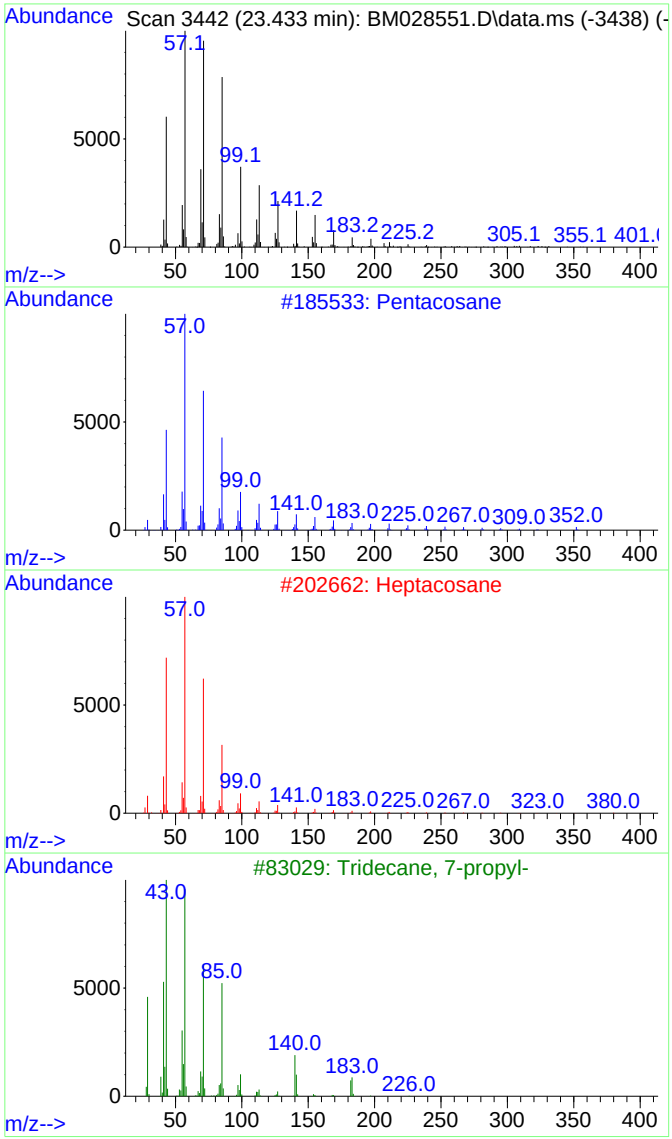
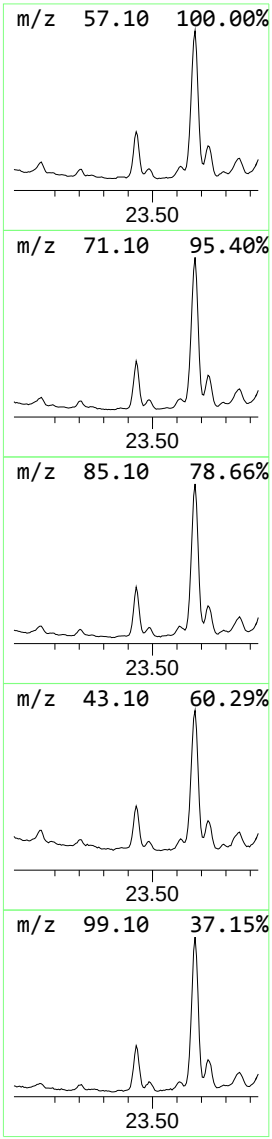
Peak Number 16 Tridecane, 7-propyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.433	26.75 ng	409411	Perylene-d12	23.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	90
2	Heptacosane	380	C27H56	000593-49-7	90
3	Tridecane, 7-propyl-	226	C16H34	055045-09-5	68
4	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	64
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
Data File : BM028551.D
Acq On : 26 Jan 2021 21:22
Operator : CG/JU
Sample : M1217-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1617

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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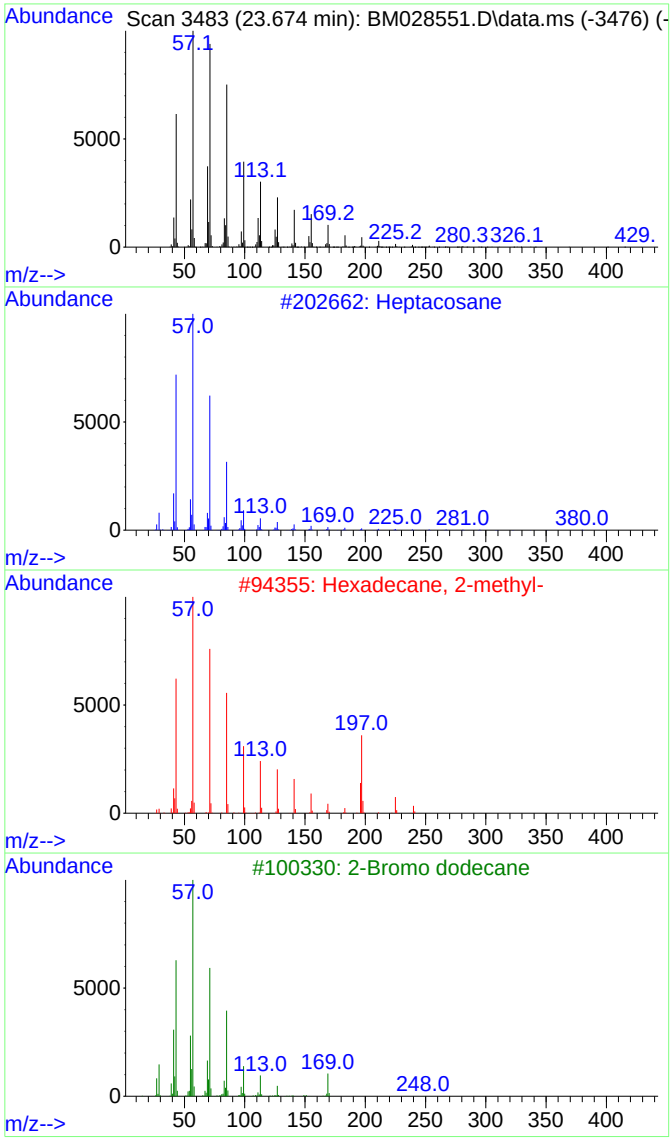
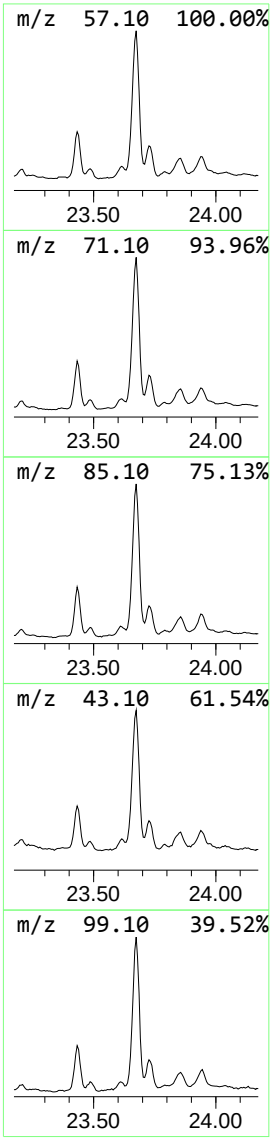
Peak Number 17 unknown23.674 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.674	116.63 ng	1784700	Perylene-d12	23.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	86
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	58
4	Tridecane, 7-propyl-	226	C16H34	055045-09-5	58
5	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	58





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Data File : BM028551.D
Acq On : 26 Jan 2021 21:22
Operator : CG/JU
Sample : M1217-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1617

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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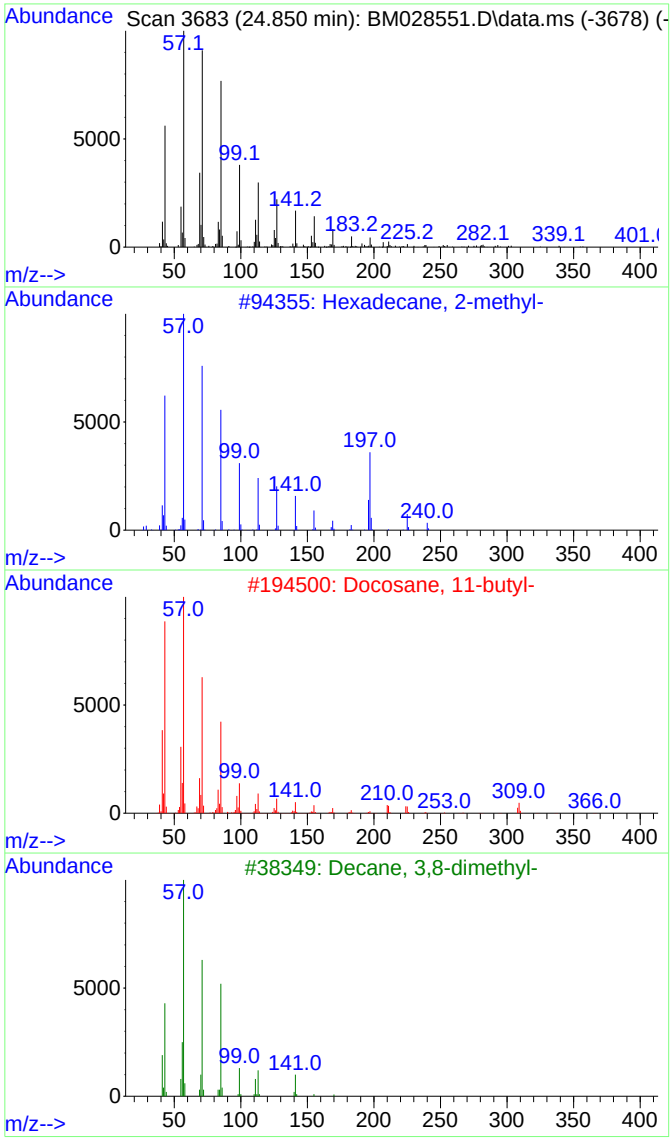
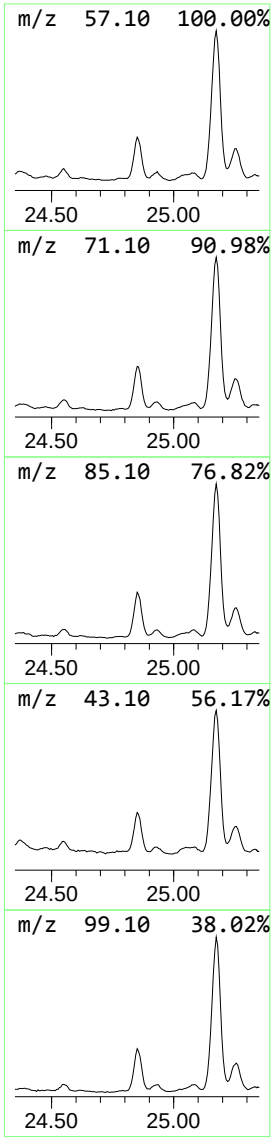
Peak Number 18 Docosane, 11-butyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.850	27.84 ng	426054	Perylene-d12	23.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	90
2	Docosane, 11-butyl-	366	C26H54	013475-76-8	83
3	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	72
4	Hentriacontane	437	C31H64	000630-04-6	64
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
Data File : BM028551.D
Acq On : 26 Jan 2021 21:22
Operator : CG/JU
Sample : M1217-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1617

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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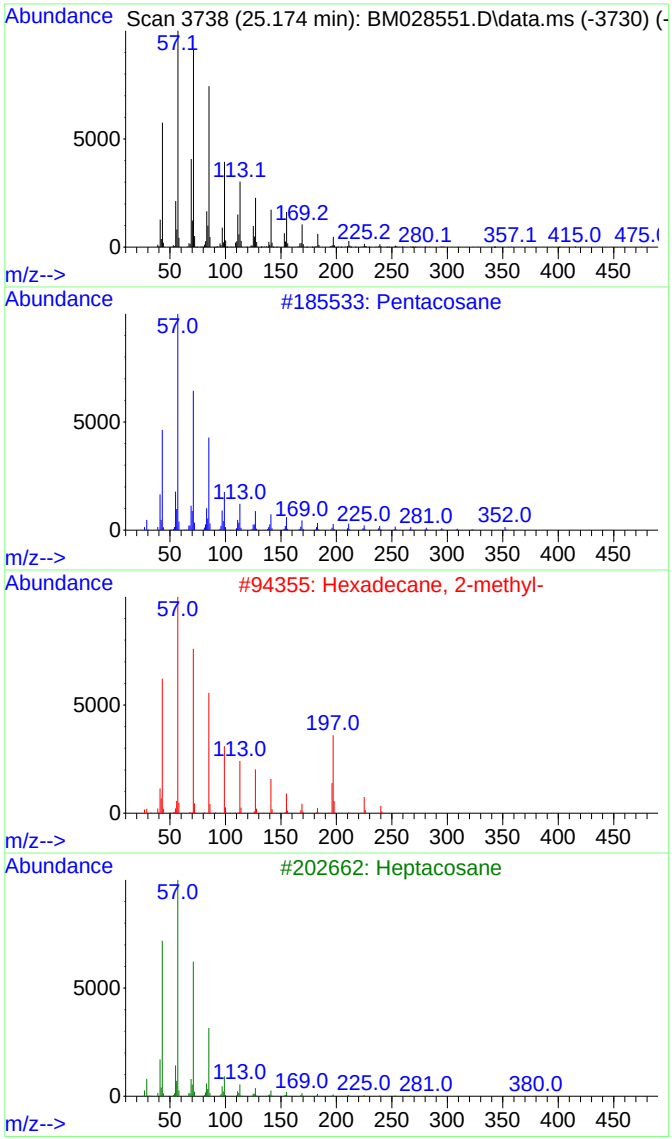
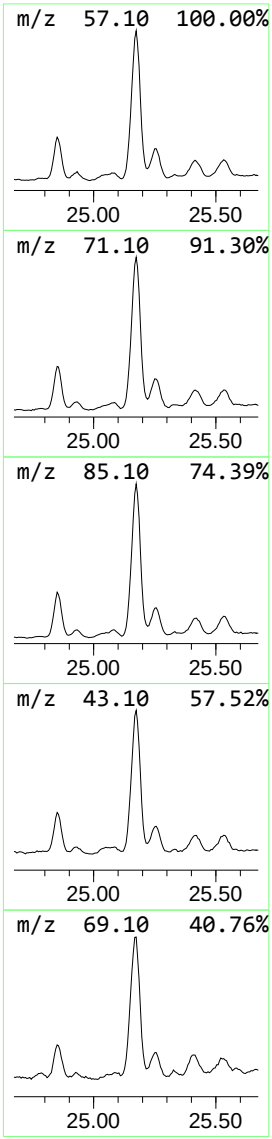
Peak Number 19 Hentriacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.174	116.17 ng	1777650	Perylene-d12	23.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	86
3	Heptacosane	380	C27H56	000593-49-7	86
4	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	68
5	Hentriacontane	437	C31H64	000630-04-6	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
Data File : BM028551.D
Acq On : 26 Jan 2021 21:22
Operator : CG/JU
Sample : M1217-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1617

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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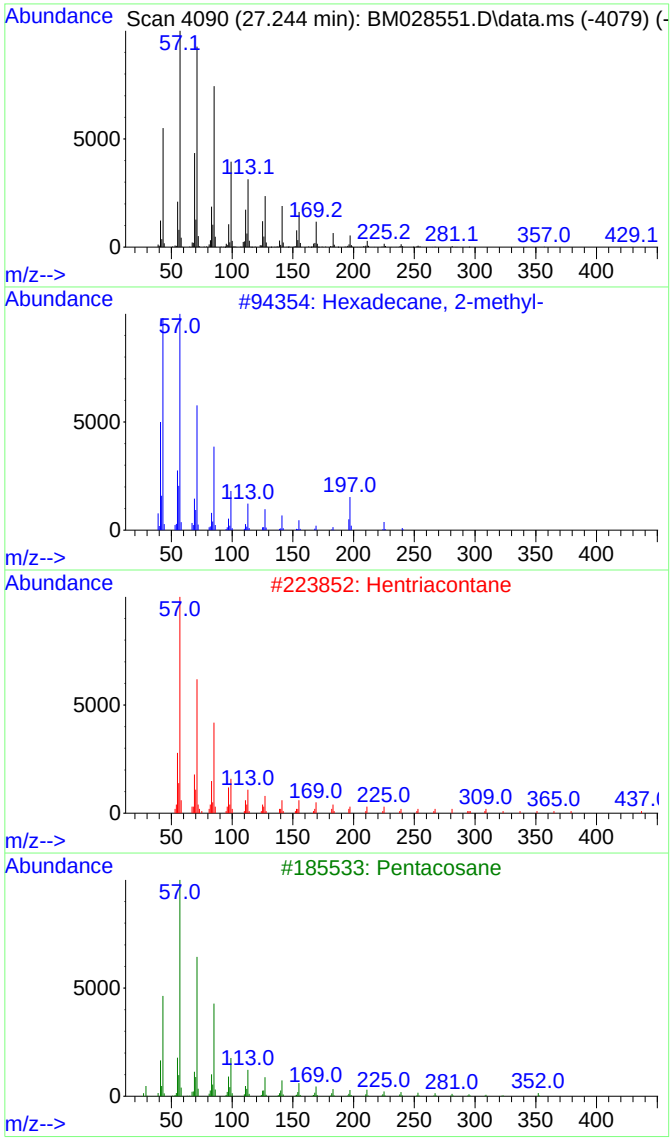
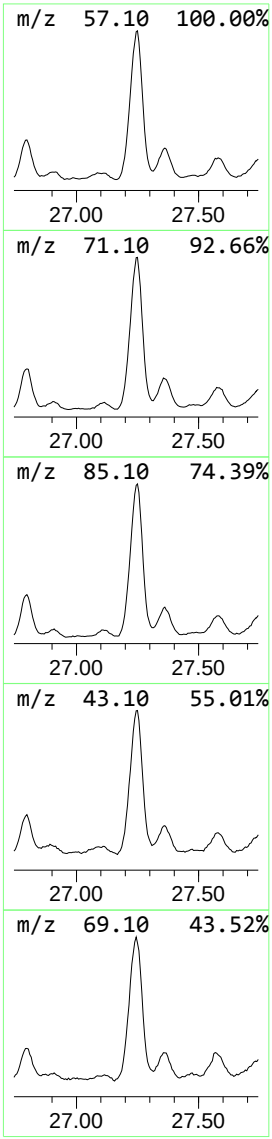
Peak Number 20 unknown27.244 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.244	121.60 ng	1860760	Perylene-d12	23.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	90
2	Hentriacontane	437	C31H64	000630-04-6	90
3	Pentacosane	352	C25H52	000629-99-2	90
4	Tridecane, 7-propyl-	226	C16H34	055045-09-5	53
5	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
Data File : BM028551.D
Acq On : 26 Jan 2021 21:22
Operator : CG/JU
Sample : M1217-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1617

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Heptacosane	14.851	42.6	ng	906597	3	14.633	425240	20.0
Heneicosane	16.333	36.9	ng	609562	4	17.362	330477	20.0
Cyclohexane, 1,...	16.574	26.0	ng	429716	4	17.362	330477	20.0
2-Bromo dodecane	16.680	64.1	ng	1058740	4	17.362	330477	20.0
unknown16.798	16.798	25.0	ng	413782	4	17.362	330477	20.0
Tetradecane, 2,...	17.939	30.7	ng	506994	4	17.362	330477	20.0
Pentacosane	18.239	135.8	ng	2243540	4	17.362	330477	20.0
Bromoacetic aci...	19.092	51.8	ng	856457	4	17.362	330477	20.0
Octadecanoic acid	19.515	75.9	ng	1079910	5	21.503	284649	20.0
Hexadecane, 2-m...	19.551	109.0	ng	1551600	5	21.503	284649	20.0
Heptadecane, 2-...	20.439	51.4	ng	731489	5	21.503	284649	20.0
Tridecane, 3-me...	20.639	83.2	ng	1184580	5	21.503	284649	20.0
Decane, 3,8-dim...	21.586	82.7	ng	1177280	5	21.503	284649	20.0
Octacosane	22.339	34.4	ng	489109	5	21.503	284649	20.0
unknown22.527	22.527	128.7	ng	1831920	5	21.503	284649	20.0
Tridecane, 7-pr...	23.433	26.8	ng	409411	6	23.774	306056	20.0
unknown23.674	23.674	116.6	ng	1784700	6	23.774	306056	20.0
Docosane, 11-bu...	24.850	27.8	ng	426054	6	23.774	306056	20.0
Hentriacontane	25.174	116.2	ng	1777650	6	23.774	306056	20.0
unknown27.244	27.244	121.6	ng	1860760	6	23.774	306056	20.0