LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050423\
Data File : BF133253.D
Acq On : 05 May 2023 02:46
Operator : CG\JU
Sample : 02598-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ETGI-328

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_F\Methods\8270-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133253.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.910	476	480	492	rVB	235734	301967	7.63%	0.932%
2	5.334	547	552	555	rBV	3964466	3746609	94.71%	11.569%
3	6.363	722	727	730	rBV	3581123	3823685	96.66%	11.807%
4	6.728	785	789	792	rBV	1371263	1161562	29.36%	3.587%
5	7.292	880	885	888	rBV	2575249	2420700	61.20%	7.475%
6	8.010	1003	1007	1010	rBV	1977347	1517357	38.36%	4.685%
7	9.086	1186	1190	1193	rBV	4846348	3955667	100.00%	12.215%
8	9.175	1200	1205	1211	rBV	75923	78771	1.99%	0.243%
9	9.698	1292	1294	1298	rVB	92602	75958	1.92%	0.235%
10	9.763	1301	1305	1308	rVB	1780544	1488886	37.64%	4.598%
11	10.198	1377	1379	1382	rVB	111504	83903	2.12%	0.259%
12	10.469	1422	1425	1429	rVB	276206	244405	6.18%	0.755%
13	10.545	1434	1438	1443	rBV	2150999	1874478	47.39%	5.788%
14	10.669	1457	1459	1467	rVB3	134296	195162	4.93%	0.603%
15	10.733	1467	1470	1473	rBV	65572	70700	1.79%	0.218%
16	10.910	1497	1500	1504	rBV4	39914	52452	1.33%	0.162%
17	10.992	1511	1514	1521	rVB5	38303	54998	1.39%	0.170%
18	11.116	1531	1535	1538	rBV2	124531	126771	3.20%	0.391%
19	11.151	1538	1541	1548	rVB3	43641	53333	1.35%	0.165%
20	11.239	1553	1556	1559	rBV	1502285	1277466	32.29%	3.945%
21	11.263	1559	1560	1563	rVV	293188	175529	4.44%	0.542%
22	11.316	1566	1569	1571	rVB2	72347	67710	1.71%	0.209%
23	11.545	1605	1608	1611	rBV	103864	81735	2.07%	0.252%
24	11.645	1622	1625	1631	rVB2	51179	55898	1.41%	0.173%
25	11.780	1644	1648	1651	rBV2	347850	370160	9.36%	1.143%
26	11.851	1657	1660	1662	rBV3	54193	58181	1.47%	0.180%
27	11.951	1674	1677	1680	rVB2	105068	87454	2.21%	0.270%
28	12.345	1738	1744	1746	rBV3	96774	167725	4.24%	0.518%
29	12.374	1746	1749	1753	rVB	55922	56454	1.43%	0.174%
30	12.451	1758	1762	1765	rBV	506549	459342	11.61%	1.418%
31	12.563	1778	1781	1786	rBV3	74385	90970	2.30%	0.281%
32	12.674	1795	1800	1803	rBV	464249	471538	11.92%	1.456%
33	12.710	1803	1806	1809	rBV2	135379	131583	3.33%	0.406%
34	12.827	1822	1826	1829	rBV	3549719	2967411	75.02%	9.163%
35	13.010	1854	1857	1859	rVB	64293	63662	1.61%	0.197%
36	13.069	1864	1867	1870	rBV2	141625	143192	3.62%	0.442%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050423\
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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-328

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_F\Methods\8270-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.345	1911	1914	1918	rVB	129783	113139	2.86%	0.349%
38	13.410	1922	1925	1928	rBV	165635	144943	3.66%	0.448%
39	13.674	1968	1970	1974	rBV3	59750	59058	1.49%	0.182%
40	13.739	1979	1981	1991	rVB2	238538	338814	8.57%	1.046%
41	13.874	1999	2004	2007	rBV2	1311921	1386669	35.06%	4.282%
42	13.898	2007	2008	2011	rVB	233606	140262	3.55%	0.433%
43	14.057	2032	2035	2038	rBV2	166200	159105	4.02%	0.491%
44	14.357	2083	2086	2089	rBV	219980	224022	5.66%	0.692%
45	14.657	2135	2137	2145	rVB2	164816	169168	4.28%	0.522%
46	14.727	2146	2149	2154	rVB	289207	275991	6.98%	0.852%
47	14.892	2174	2177	2179	rBV	171806	206029	5.21%	0.636%
48	14.980	2189	2192	2199	rVB2	212657	245628	6.21%	0.758%
49	15.233	2232	2235	2238	rBV	125064	146083	3.69%	0.451%
50	15.292	2241	2245	2249	rBV	599490	722202	18.26%	2.230%

Sum of corrected areas: 32384487

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Instrument :
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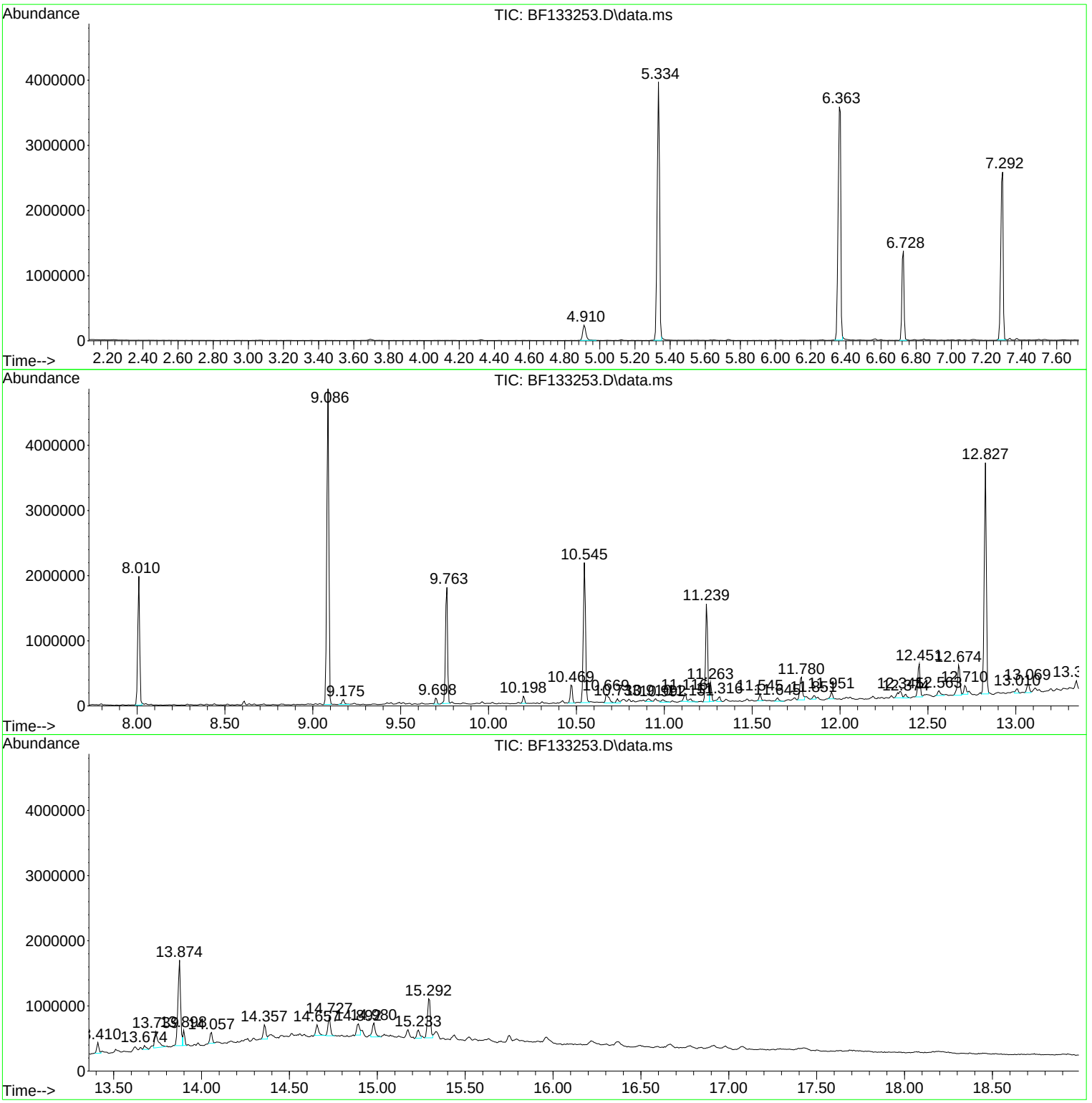
ClientSampleId :
ETGI-328

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050423\
Data File : BF133253.D
Acq On : 05 May 2023 02:46
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Sample : 02598-04
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Instrument :
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ClientSampleId :
ETGI-328

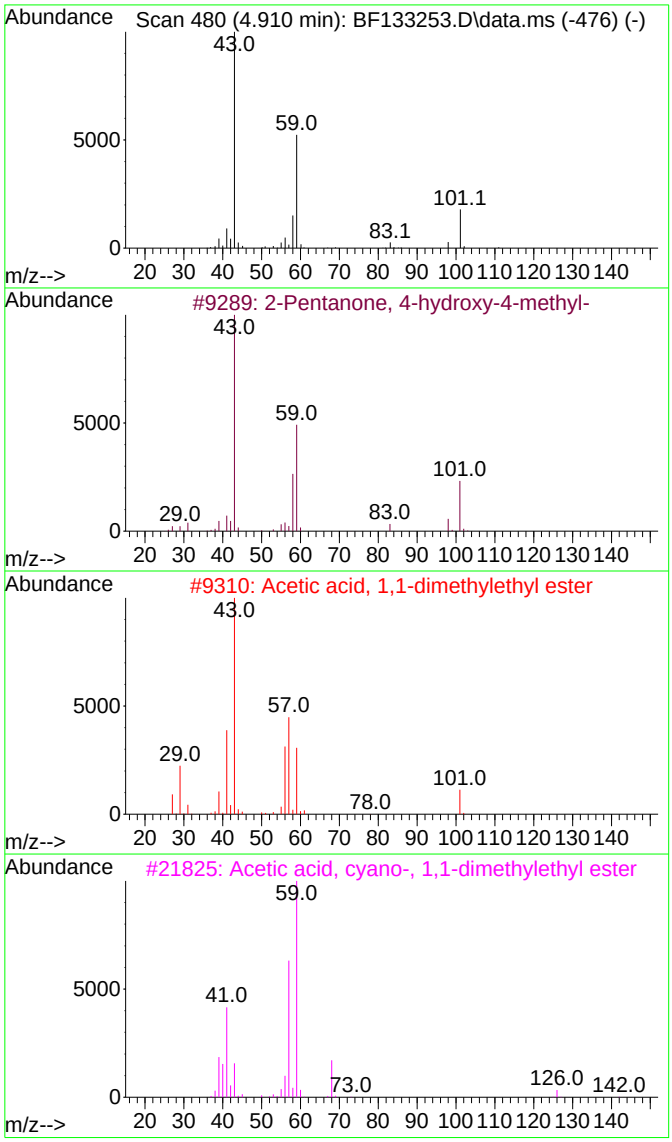
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

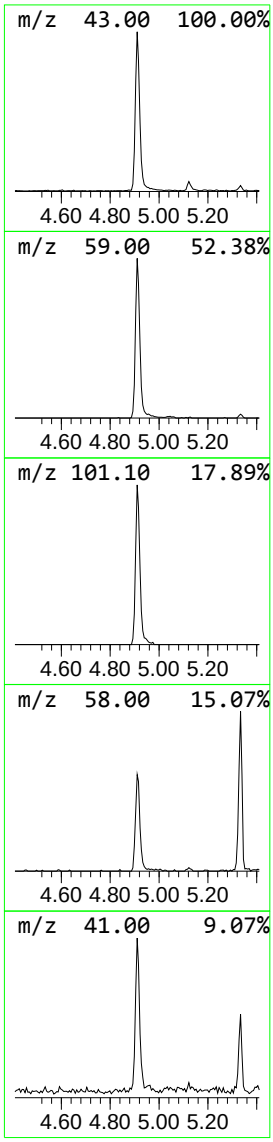
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.910	5.20 ng	301967	1,4-Dichlorobenzene-d4	6.728

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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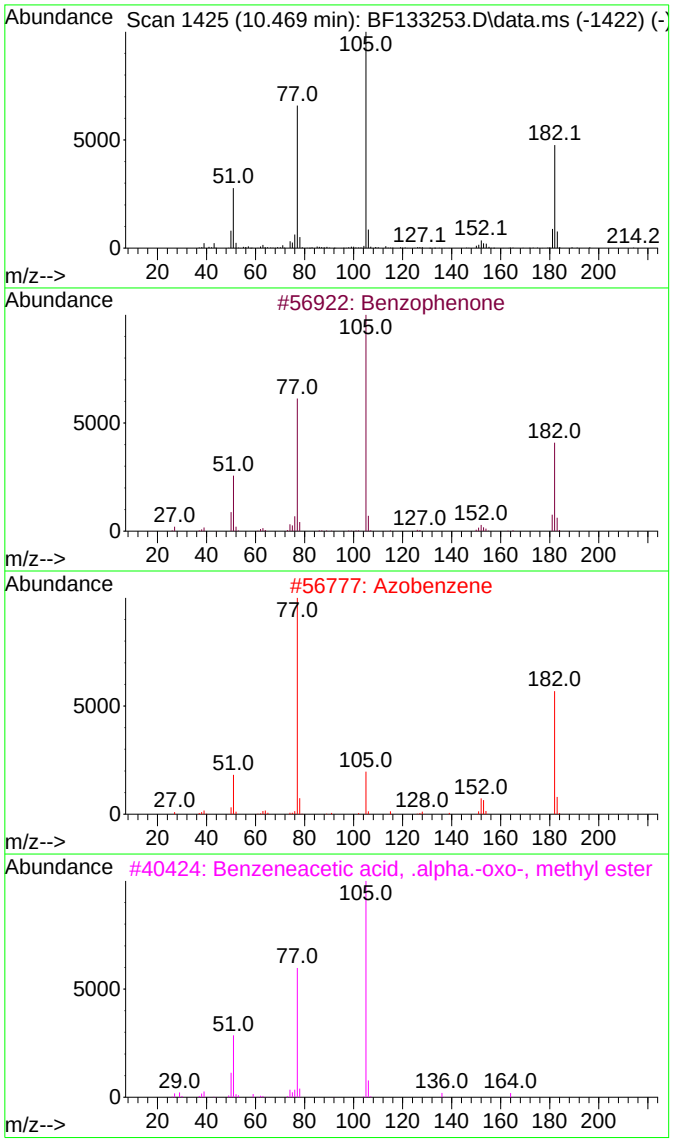
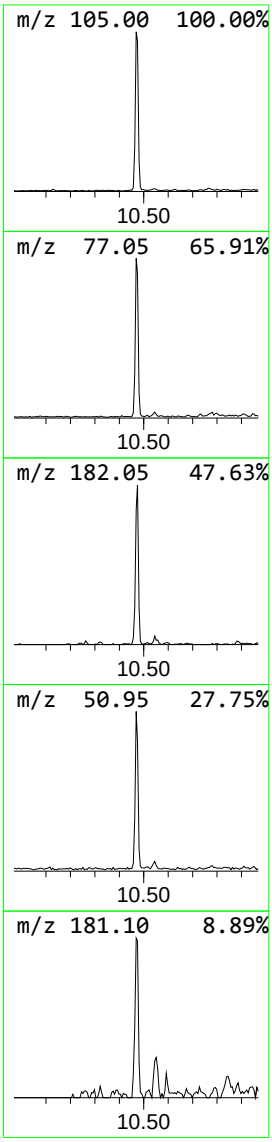
Peak Number 2 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.469	3.28 ng	244405	Acenaphthene-d10	9.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	59
3	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
4	Benzenebutanoic acid, .gamma.-ox...	192	C11H12O3	025333-24-8	47
5	N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	47





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Acq On : 05 May 2023 02:46
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Sample : 02598-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-328

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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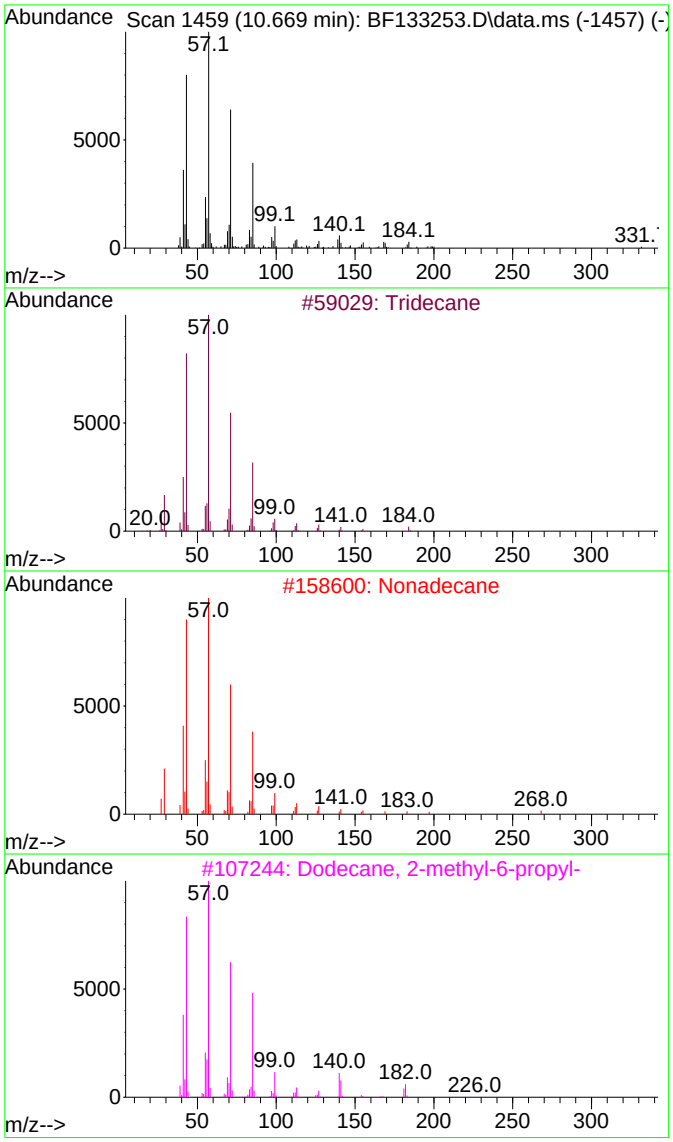
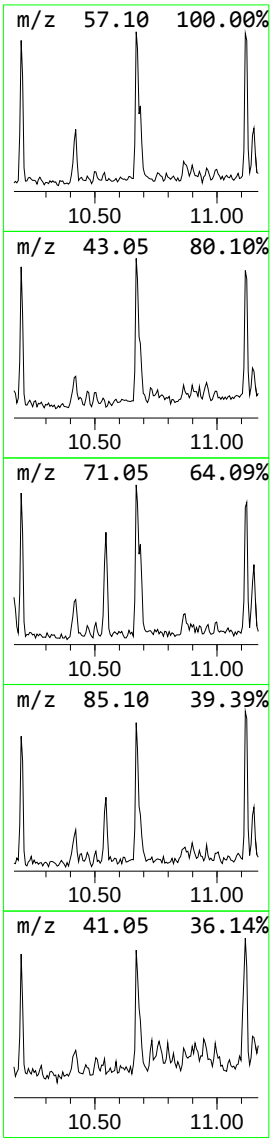
Peak Number 3 Tridecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.669	3.06 ng	195162	Phenanthrene-d10	11.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	96
2	Nonadecane	268	C19H40	000629-92-5	87
3	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
4	Pentadecane	212	C15H32	000629-62-9	86
5	Heptadecane	240	C17H36	000629-78-7	86





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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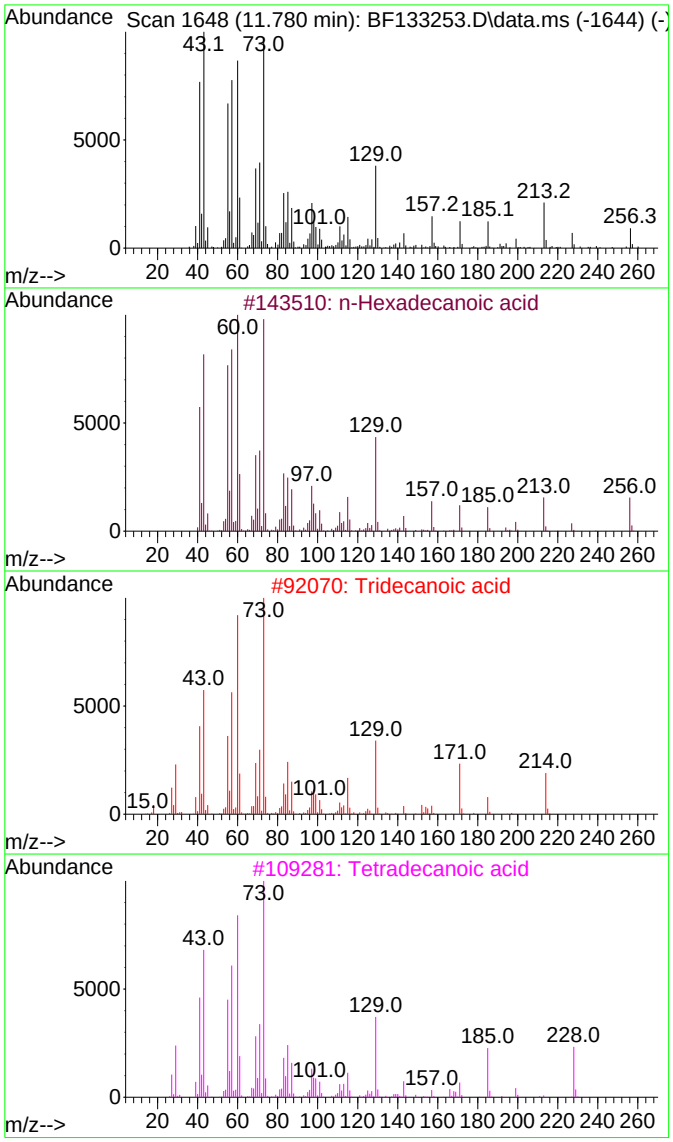
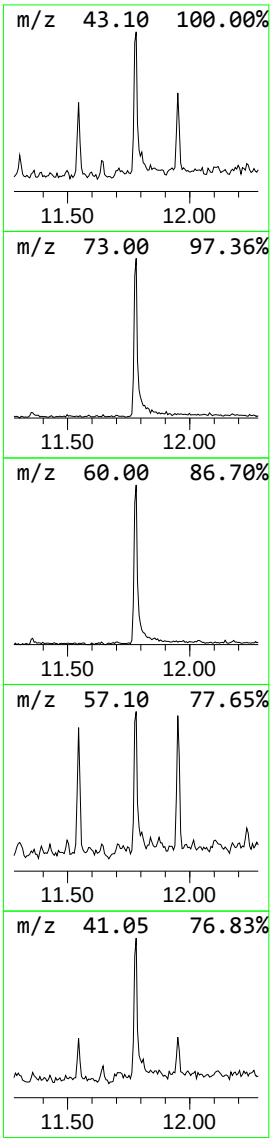
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.780	5.80 ng	370160	Phenanthrene-d10	11.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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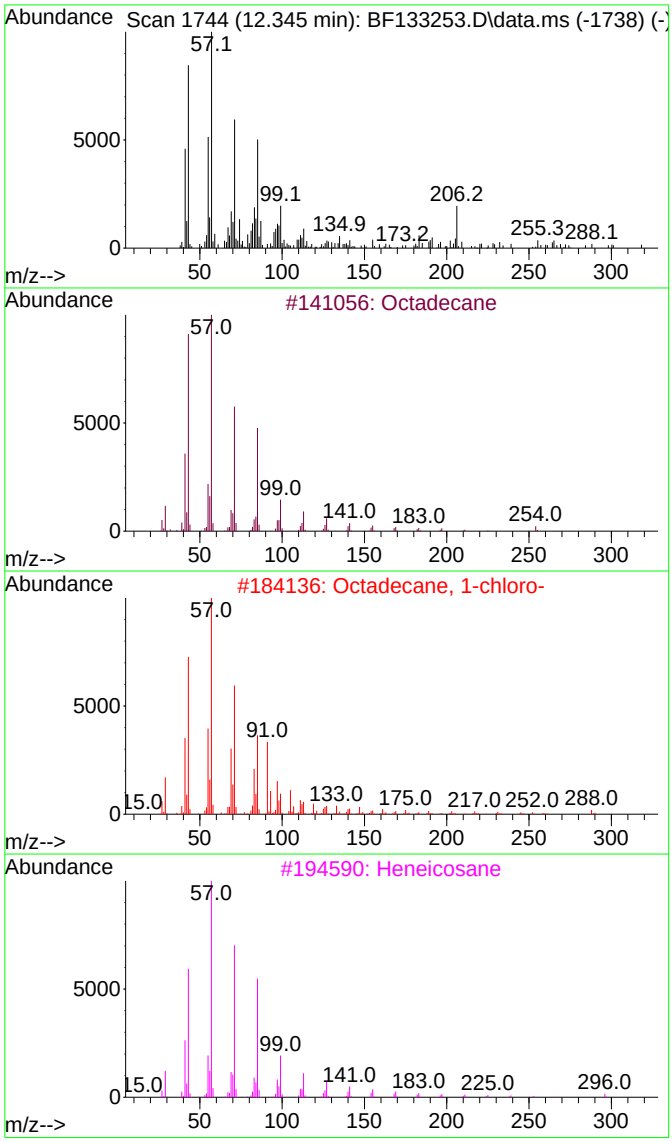
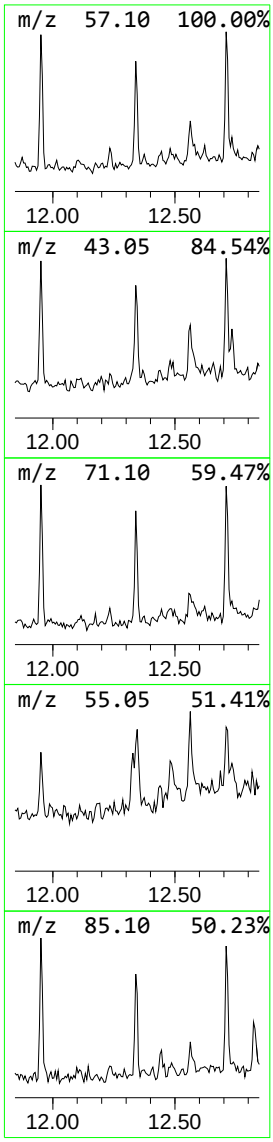
Peak Number 5 Octadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.345	2.63 ng	167725	Phenanthrene-d10	11.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	70
2	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	70
3	Heneicosane	296	C21H44	000629-94-7	68
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	64
5	10-Methylnonadecane	282	C20H42	056862-62-5	64





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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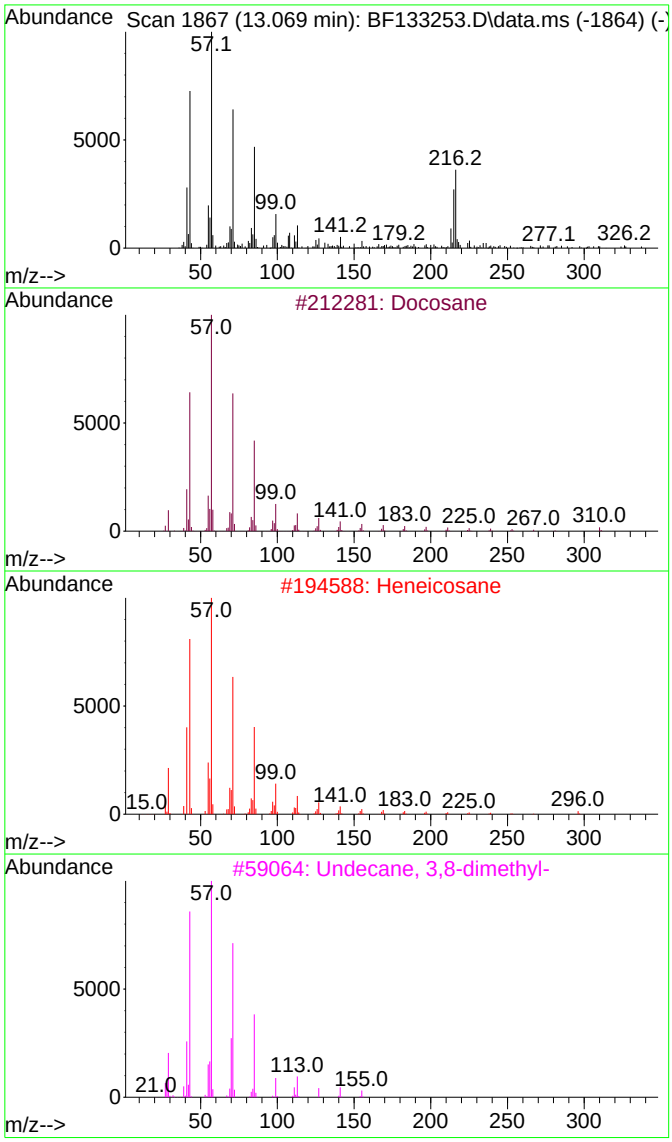
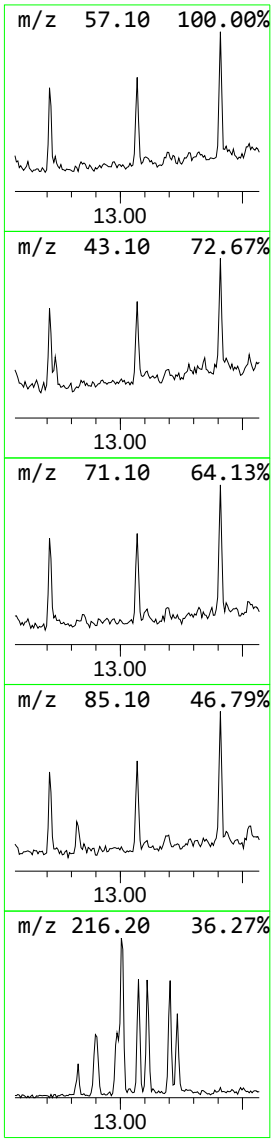
Peak Number 6 Docosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.069	2.07 ng	143192	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	83
2	Heneicosane	296	C21H44	000629-94-7	64
3	Undecane, 3,8-dimethyl-	184	C13H28	017301-30-3	58
4	Heptadecane	240	C17H36	000629-78-7	58
5	Octadecane	254	C18H38	000593-45-3	58





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Misc :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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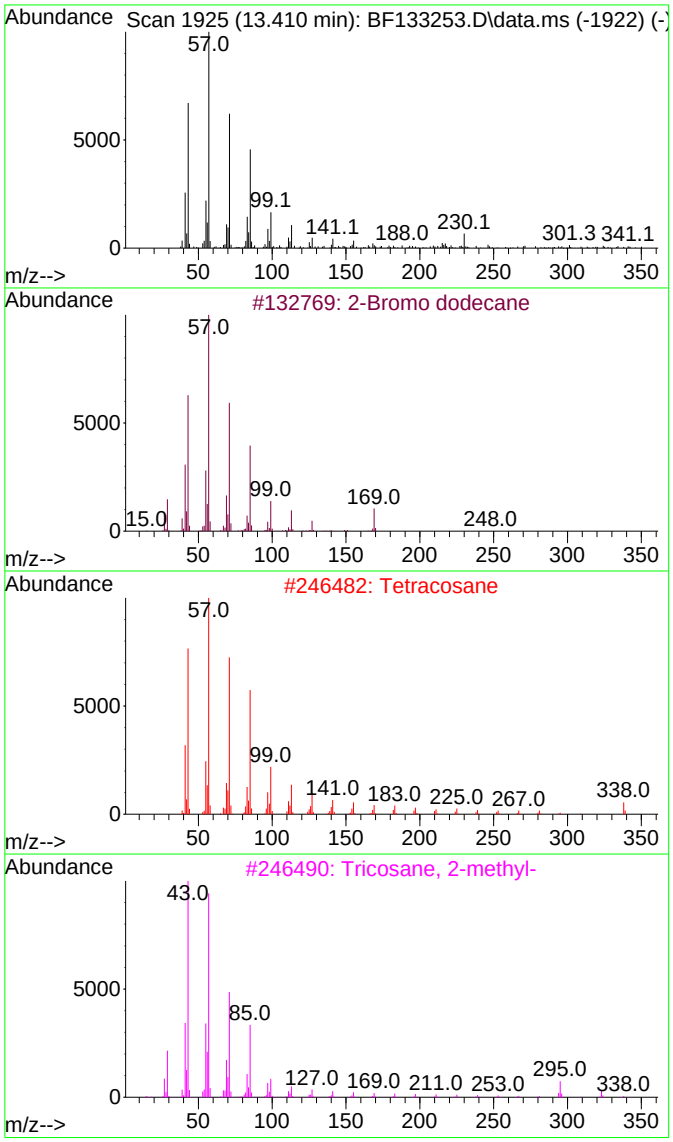
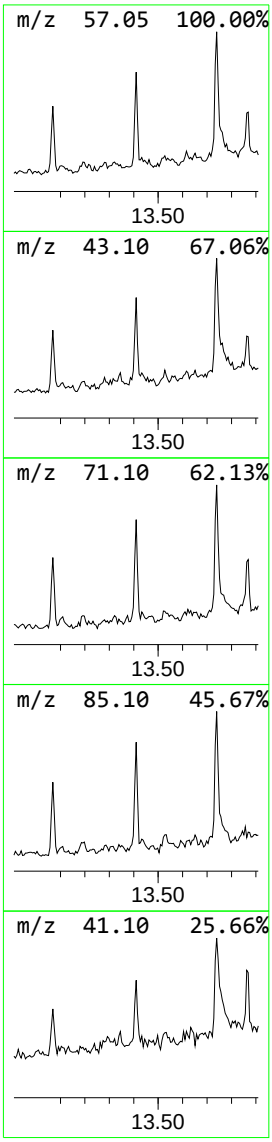
Peak Number 7 2-Bromo dodecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.410	2.09 ng	144943	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Tricosane, 2-methyl-	338	C24H50	001928-30-9	87
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	87
5	Hexacosane	366	C26H54	000630-01-3	83





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Data File : BF133253.D
Acq On : 05 May 2023 02:46
Operator : CG\JU
Sample : 02598-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-328

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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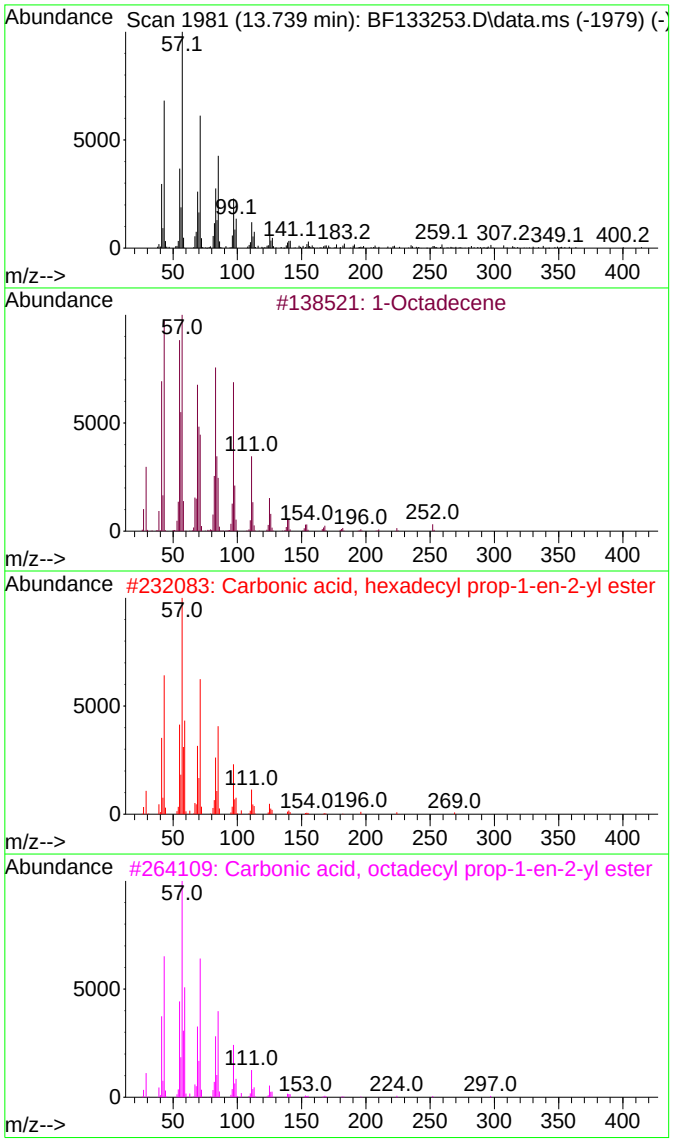
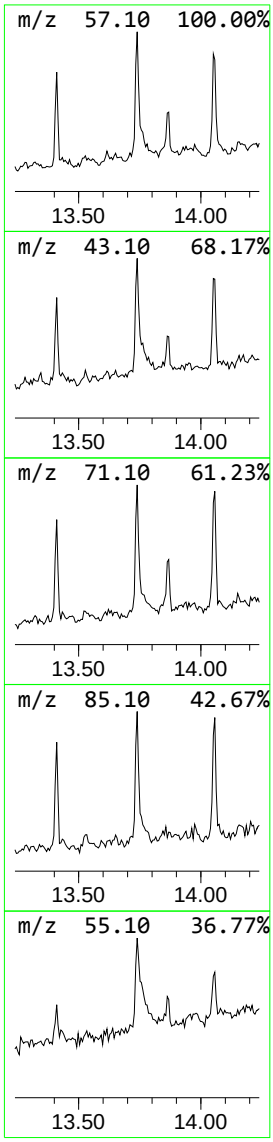
Peak Number 8 1-Octadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.739	4.89 ng	338814	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	95
2	Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	91
3	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	91
4	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	91
5	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	91





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Acq On : 05 May 2023 02:46
Operator : CG\JU
Sample : 02598-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-328

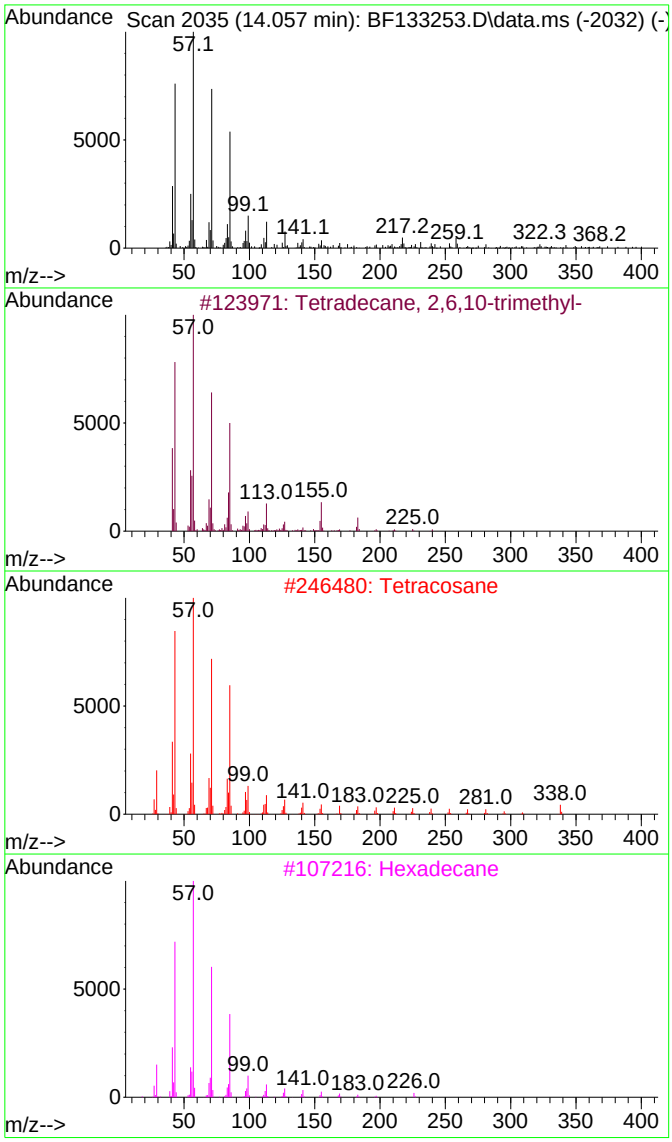
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

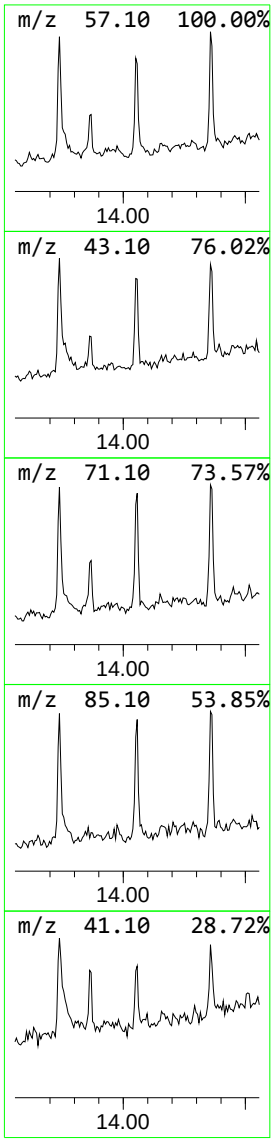
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Tetradecane, 2,6,10-trimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.057	2.29 ng	159105	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	90
2	Tetracosane	338	C24H50	000646-31-1	87
3	Hexadecane	226	C16H34	000544-76-3	87
4	Heptadecane	240	C17H36	000629-78-7	87
5	Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	87





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Operator : CG\JU
Sample : 02598-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-328

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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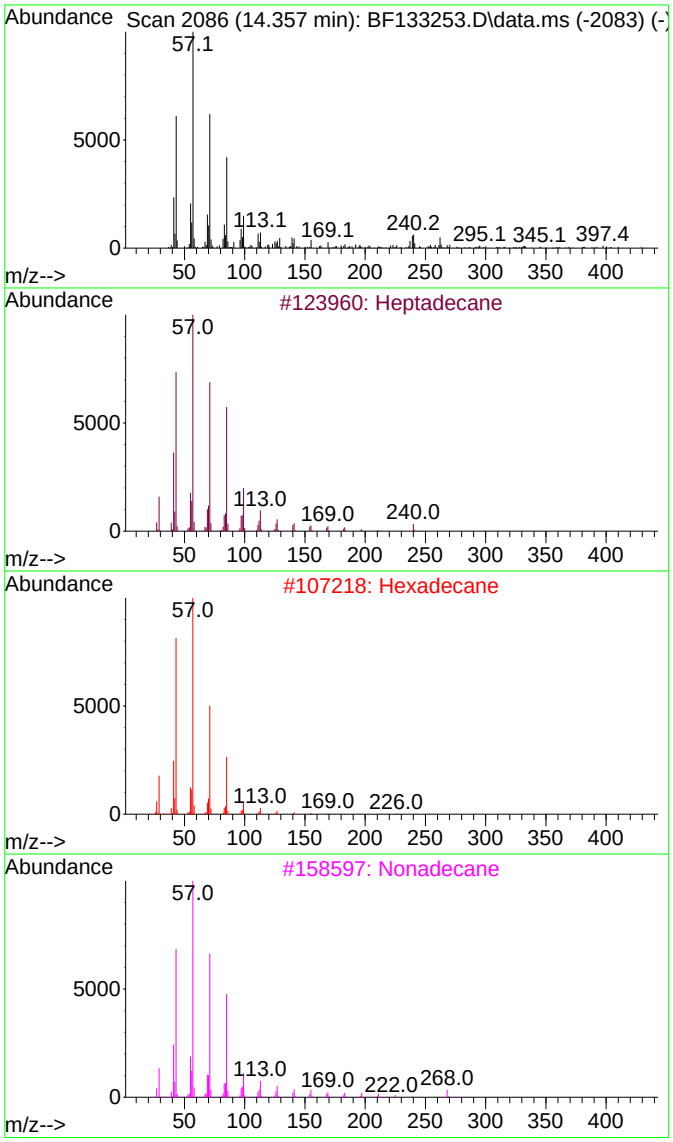
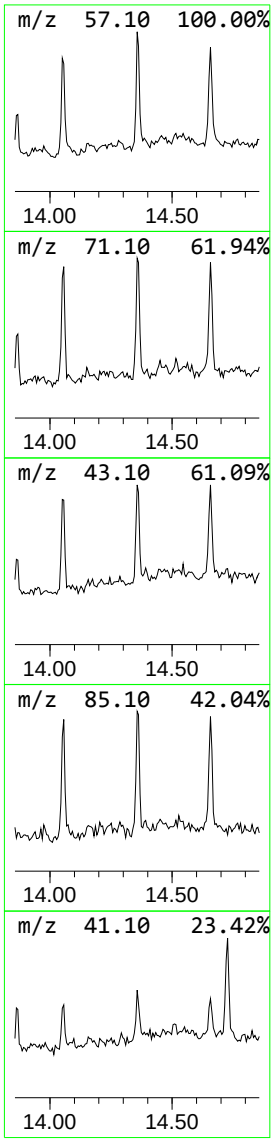
Peak Number 10 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.357	3.23 ng	224022	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	95
2	Hexadecane	226	C16H34	000544-76-3	95
3	Nonadecane	268	C19H40	000629-92-5	94
4	Docosane	310	C22H46	000629-97-0	93
5	Octadecane	254	C18H38	000593-45-3	91





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Operator : CG\JU
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ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
ETGI-328

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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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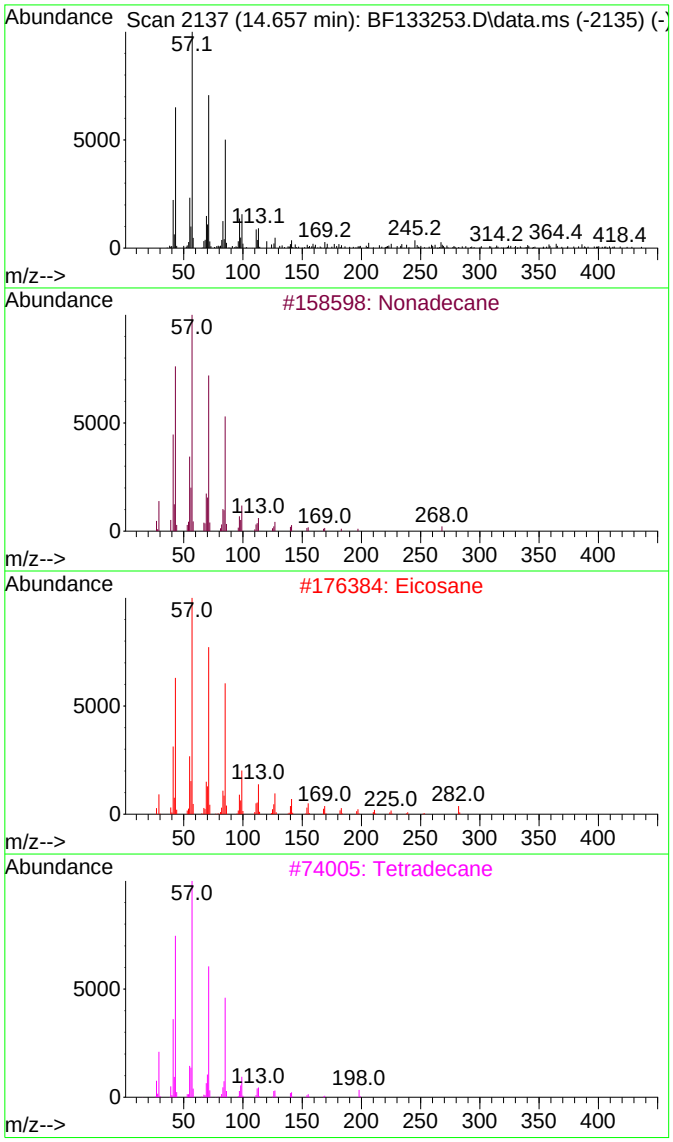
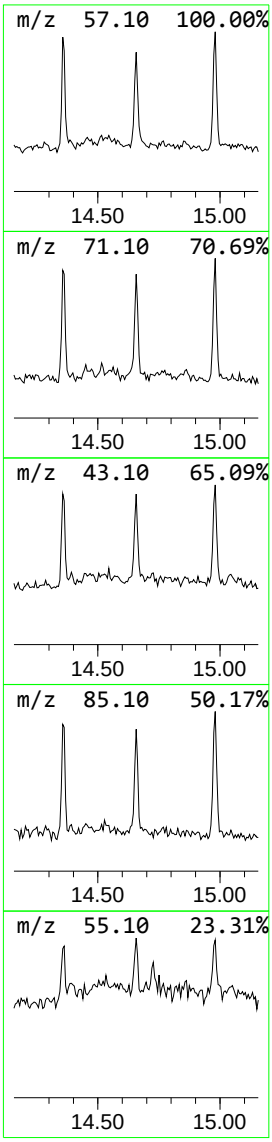
Peak Number 11 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.657	4.68 ng	169168	Perylene-d12	15.298

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Tetradecane	198	C14H30	000629-59-4	90
4	Hentriacontane	437	C31H64	000630-04-6	89
5	Octacosane	394	C28H58	000630-02-4	87





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Acq On : 05 May 2023 02:46
Operator : CG\JU
Sample : 02598-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-328

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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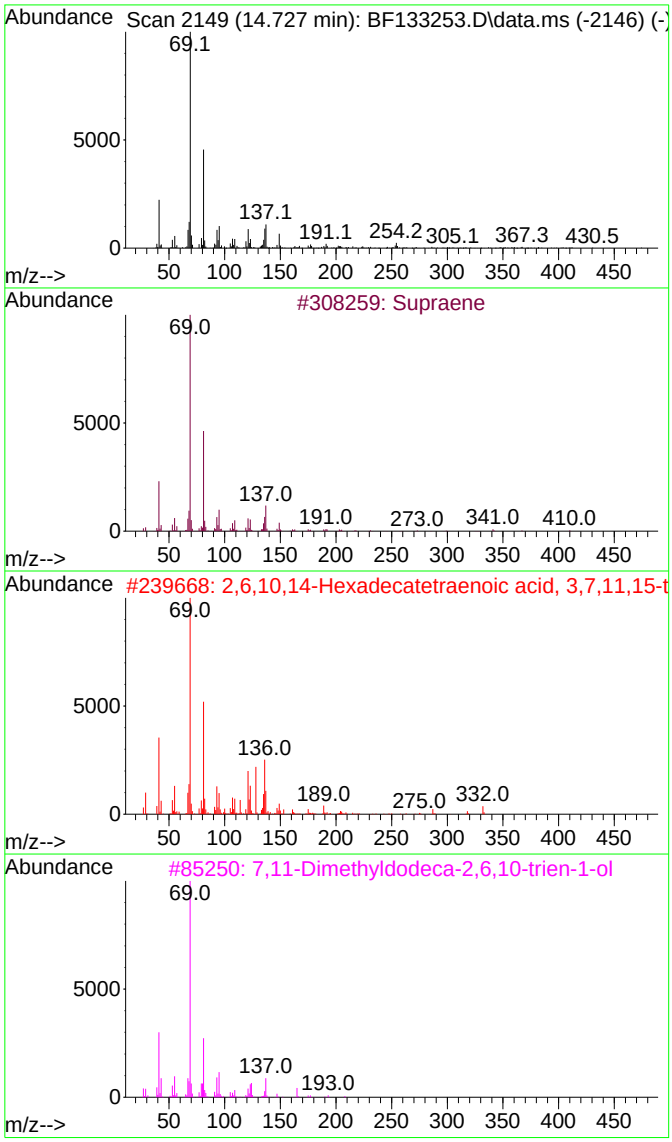
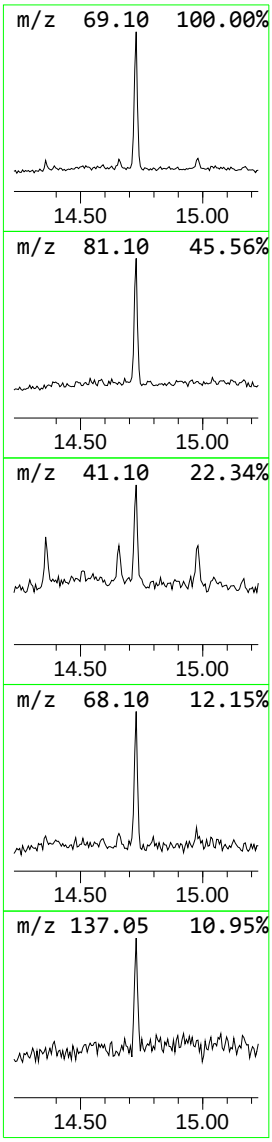
Peak Number 12 Supraene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.727	7.64 ng	275991	Perylene-d12	15.298

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	90
2	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59
4	5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	59
5	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	58





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Operator : CG\JU
Sample : 02598-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-328

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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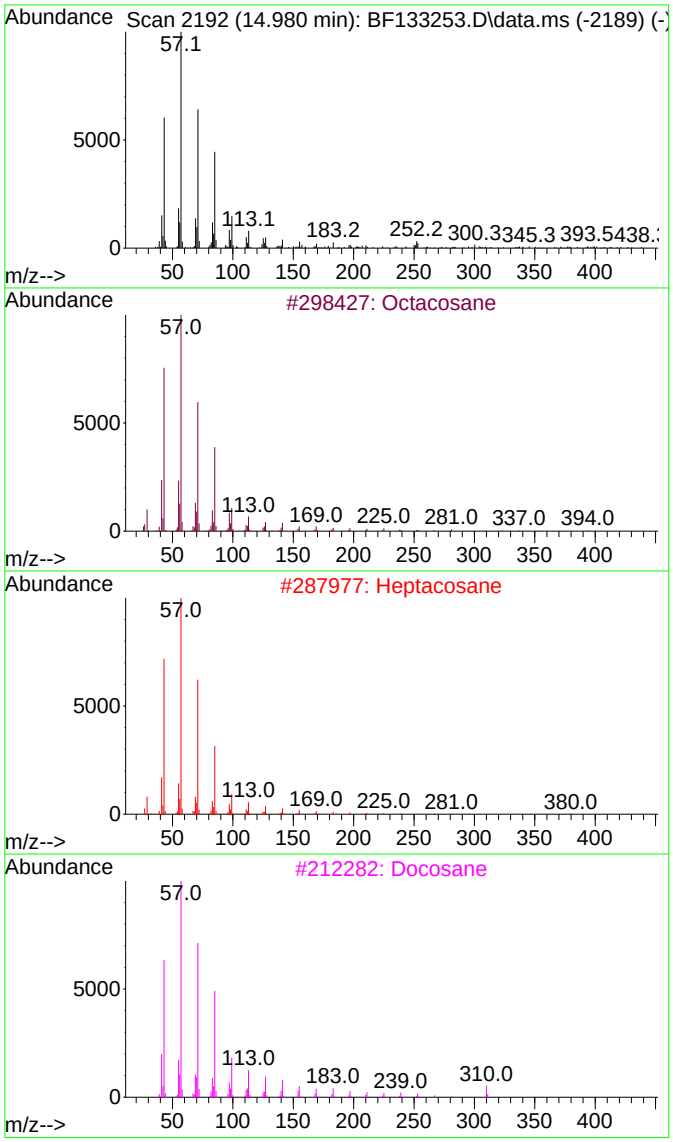
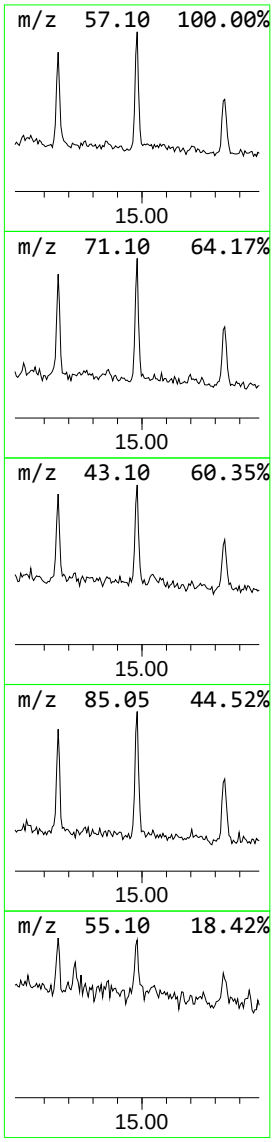
Peak Number 13 Octacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.980	6.80 ng	245628	Perylene-d12	15.298

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	99
2	Heptacosane	380	C27H56	000593-49-7	96
3	Docosane	310	C22H46	000629-97-0	96
4	Hexacosane	366	C26H54	000630-01-3	87
5	Tricosane	324	C23H48	000638-67-5	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050423\
Data File : BF133253.D
Acq On : 05 May 2023 02:46
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Misc :
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Instrument :
BNA_F
ClientSampleId :
ETGI-328

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	4.910	5.2	ng	301967	1	6.728	1161560	20.0
Benzophenone	10.469	3.3	ng	244405	3	9.763	1488890	20.0
Tridecane	10.669	3.1	ng	195162	4	11.239	1277470	20.0
n-Hexadecanoic ...	11.780	5.8	ng	370160	4	11.239	1277470	20.0
Octadecane	12.345	2.6	ng	167725	4	11.239	1277470	20.0
Docosane	13.069	2.1	ng	143192	5	13.874	1386670	20.0
2-Bromo dodecane	13.410	2.1	ng	144943	5	13.874	1386670	20.0
1-Octadecene	13.739	4.9	ng	338814	5	13.874	1386670	20.0
Tetradecane, 2,...	14.057	2.3	ng	159105	5	13.874	1386670	20.0
Heptadecane	14.357	3.2	ng	224022	5	13.874	1386670	20.0
Nonadecane	14.657	4.7	ng	169168	6	15.298	722202	20.0
Supraene	14.727	7.6	ng	275991	6	15.298	722202	20.0
Octacosane	14.980	6.8	ng	245628	6	15.298	722202	20.0