LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138375.D
Acq On : 27 Jun 2024 19:39
Operator : CG\JU
Sample : P3053-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1A

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-BF061224.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138375.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	8	15	20	rVB	2019169	2595903	75.12%	5.785%
2	2.281	28	33	37	rBV	36157	43580	1.26%	0.097%
3	3.399	219	223	233	rBV	94705	176630	5.11%	0.394%
4	3.499	233	240	259	rVB	11512	51674	1.50%	0.115%
5	5.098	508	512	521	rVB	230399	253241	7.33%	0.564%
6	5.504	577	581	585	rBV	3395567	3386691	98.00%	7.547%
7	6.516	748	753	756	rBV	3764832	3288137	95.15%	7.328%
8	6.704	782	785	790	rBV	76580	64964	1.88%	0.145%
9	6.881	811	815	818	rBV	1658278	1306233	37.80%	2.911%
10	7.440	905	910	913	rBV	2511479	2190051	63.37%	4.881%
11	7.692	949	953	959	rVB	136468	105150	3.04%	0.234%
12	8.157	1029	1032	1036	rVB	1925972	1582980	45.81%	3.528%
13	8.375	1063	1069	1073	rBV	62539	58239	1.69%	0.130%
14	8.469	1081	1085	1094	rBV	296284	264289	7.65%	0.589%
15	9.234	1211	1215	1218	rBV	4362995	3455865	100.00%	7.701%
16	9.910	1327	1330	1333	rBV	1880239	1496420	43.30%	3.335%
17	9.939	1333	1335	1338	rVB2	65304	61746	1.79%	0.138%
18	10.004	1342	1346	1349	rBV2	114707	158309	4.58%	0.353%
19	10.698	1460	1464	1468	rBV	2133038	1693058	48.99%	3.773%
20	10.816	1481	1484	1491	rVB3	41692	57907	1.68%	0.129%
21	11.398	1579	1583	1585	rBV	1446314	1193942	34.55%	2.661%
22	11.422	1585	1587	1589	rVV	219553	170500	4.93%	0.380%
23	11.451	1589	1592	1594	rVV	97157	86934	2.52%	0.194%
24	11.475	1594	1596	1599	rVB	59390	48053	1.39%	0.107%
25	11.886	1662	1666	1669	rBV3	80540	98811	2.86%	0.220%
26	11.922	1669	1672	1684	rVV2	655470	662874	19.18%	1.477%
27	12.069	1694	1697	1699	rBV2	53374	49665	1.44%	0.111%
28	12.092	1699	1701	1704	rVV	85008	65080	1.88%	0.145%
29	12.539	1773	1777	1783	rBV	457662	484951	14.03%	1.081%
30	12.610	1786	1789	1791	rBV	364967	344952	9.98%	0.769%
31	12.704	1802	1805	1812	rBV2	176443	199186	5.76%	0.444%
32	12.798	1818	1821	1823	rBV	131193	115659	3.35%	0.258%
33	12.839	1825	1828	1832	rVB	238516	238780	6.91%	0.532%
34	12.980	1848	1852	1855	rBV	3294587	2669529	77.25%	5.949%
35	13.210	1888	1891	1893	rBV	60870	50114	1.45%	0.112%
36	13.363	1914	1917	1918	rBV	41498	43883	1.27%	0.098%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138375.D
Acq On : 27 Jun 2024 19:39
Operator : CG\JU
Sample : P3053-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1A

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-BF061224.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.380	1918	1920	1923	rVV3	103061	105954	3.07%	0.236%
38	13.427	1923	1928	1931	rVB2	126958	154421	4.47%	0.344%
39	13.504	1936	1941	1944	rVB3	162126	202427	5.86%	0.451%
40	13.551	1947	1949	1951	rVB	62075	45141	1.31%	0.101%
41	13.810	1991	1993	1996	rBV2	34909	49258	1.43%	0.110%
42	13.874	2000	2004	2015	rVB2	361571	500888	14.49%	1.116%
43	14.033	2026	2031	2034	rBV	1481744	1387462	40.15%	3.092%
44	14.057	2034	2035	2039	rVB	130658	79835	2.31%	0.178%
45	14.198	2056	2059	2063	rVB	86811	81525	2.36%	0.182%
46	14.504	2107	2111	2119	rBV2	438117	658641	19.06%	1.468%
47	14.810	2160	2163	2166	rVB2	92615	94249	2.73%	0.210%
48	14.886	2170	2176	2180	rVB	829327	877089	25.38%	1.955%
49	15.033	2198	2201	2205	rBV2	86724	131008	3.79%	0.292%
50	15.074	2205	2208	2211	rBV	81468	122317	3.54%	0.273%
51	15.151	2217	2221	2224	rBV	1130123	1170367	33.87%	2.608%
52	15.180	2224	2226	2231	rVB2	112119	127104	3.68%	0.283%
53	15.410	2263	2265	2267	rBV2	48312	47766	1.38%	0.106%
54	15.504	2276	2281	2285	rBV	764396	967166	27.99%	2.155%
55	15.862	2340	2342	2351	rVB3	73317	107064	3.10%	0.239%
56	15.974	2356	2361	2366	rBV	820831	1182566	34.22%	2.635%
57	16.033	2367	2371	2379	rVB2	117213	210840	6.10%	0.470%
58	16.245	2403	2407	2421	rVB	321346	620861	17.97%	1.384%
59	17.162	2559	2563	2575	rVB10	94539	228923	6.62%	0.510%
60	17.580	2627	2634	2646	rBV3	697182	2010241	58.17%	4.480%
61	17.804	2667	2672	2681	rVB2	269442	580660	16.80%	1.294%
62	18.051	2706	2714	2726	rBV	765929	2217568	64.17%	4.942%
63	18.404	2766	2774	2793	rBV6	371541	1746237	50.53%	3.891%
64	18.551	2794	2799	2805	rBV3	154709	351718	10.18%	0.784%

Sum of corrected areas: 44873276

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
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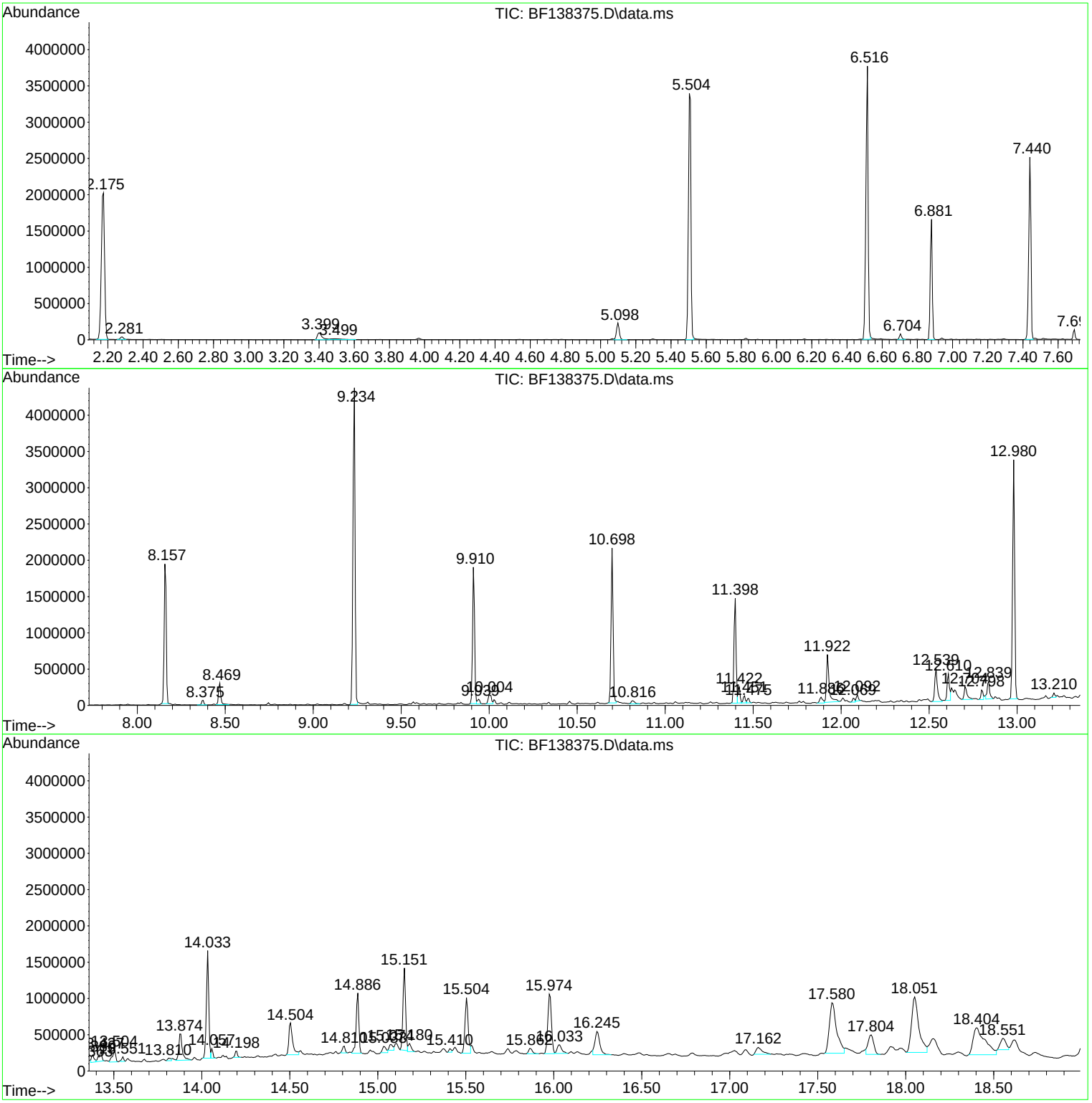
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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\BF062724\
Data File : BF138375.D
Acq On : 27 Jun 2024 19:39
Operator : CG\JU
Sample : P3053-01
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1A

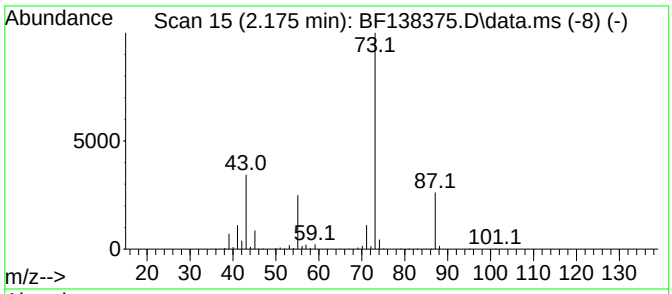
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

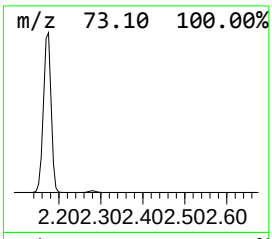
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

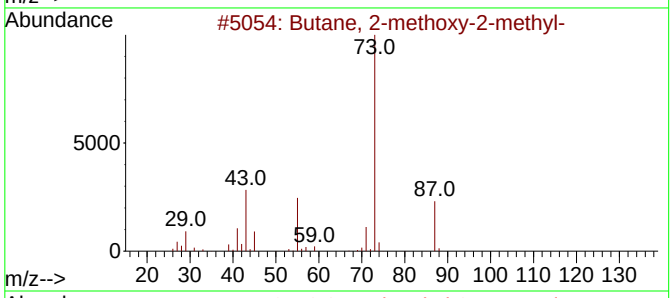
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

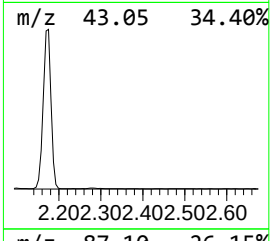
R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	39.75 ng	2595900	1,4-Dichlorobenzene-d4	6.881

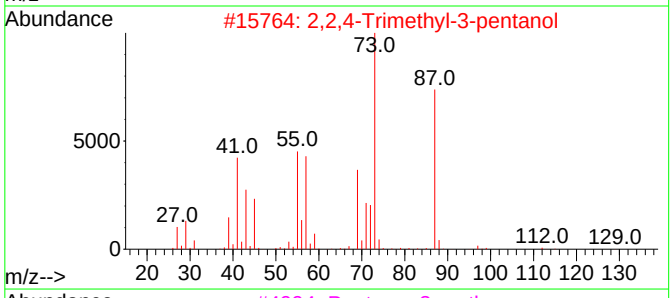
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9

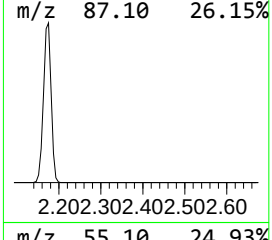


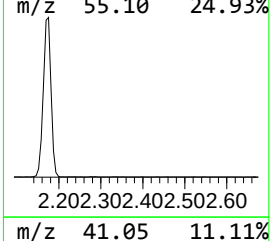


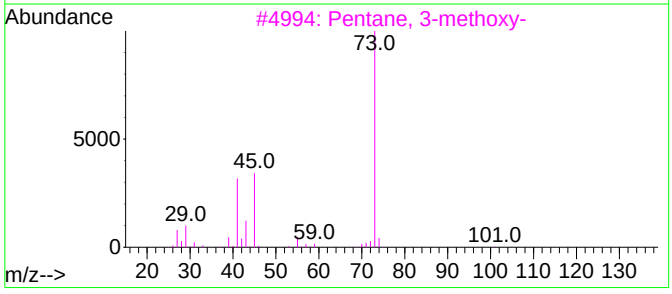


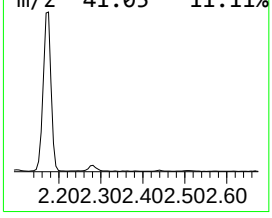












Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138375.D
Acq On : 27 Jun 2024 19:39
Operator : CG\JU
Sample : P3053-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1A

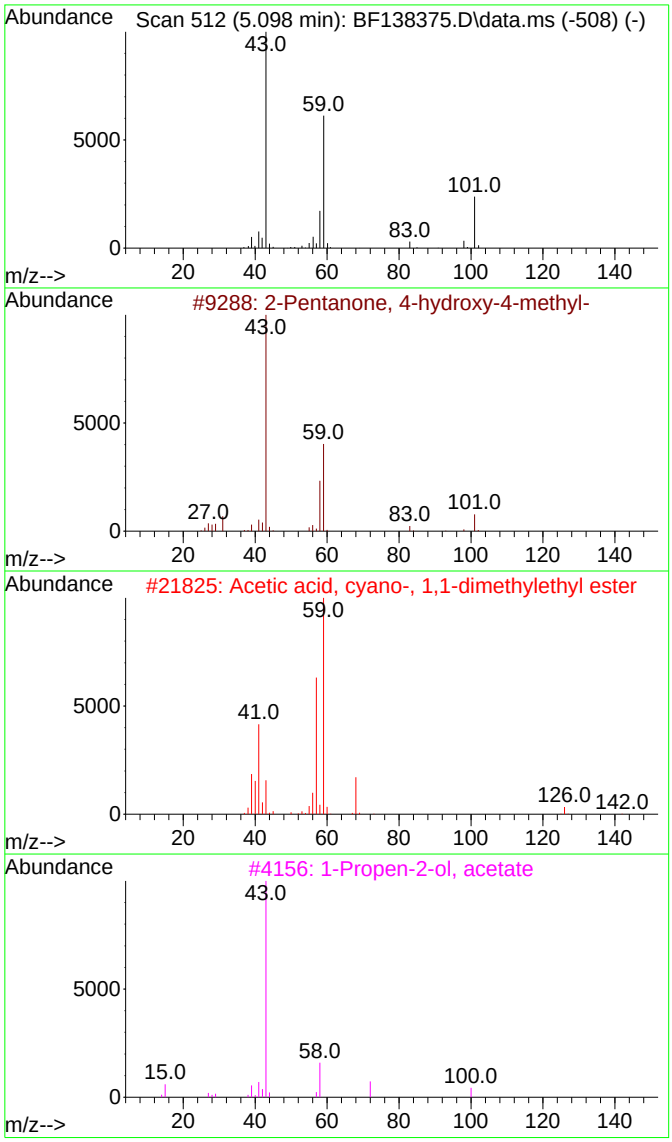
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

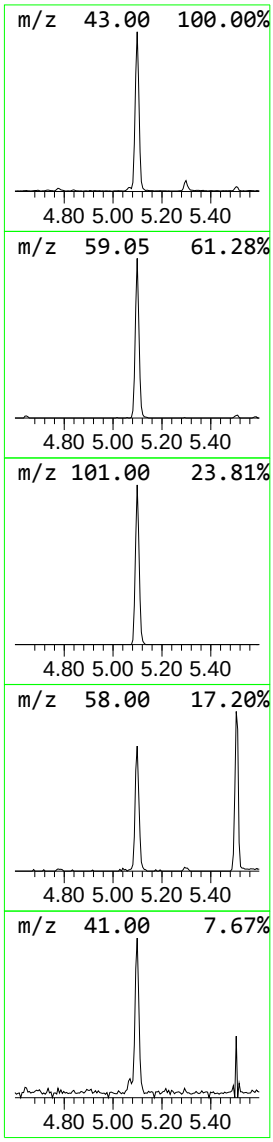
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	3.88 ng	253241	1,4-Dichlorobenzene-d4	6.881

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Guanidine	59	CH5N3	000113-00-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

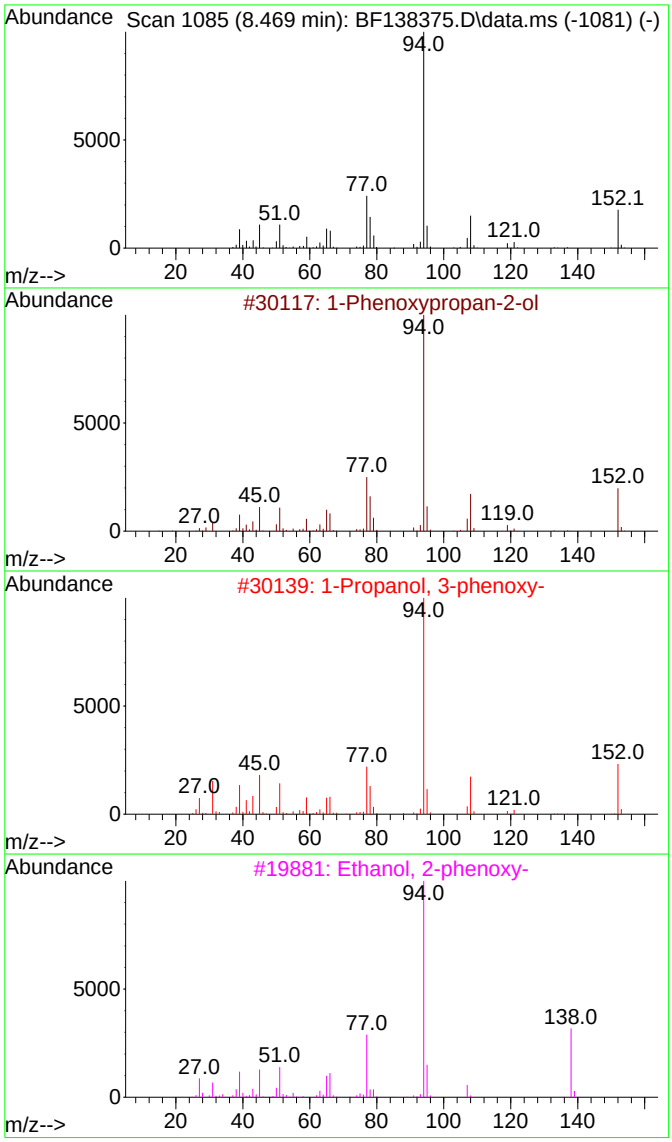
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

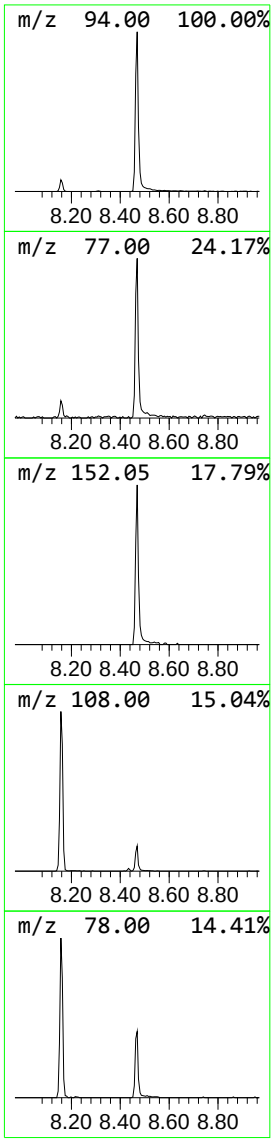
****

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.469	3.34 ng	264289	Naphthalene-d8	8.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	90
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
5	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
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ALS Vial : 15 Sample Multiplier: 1

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BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

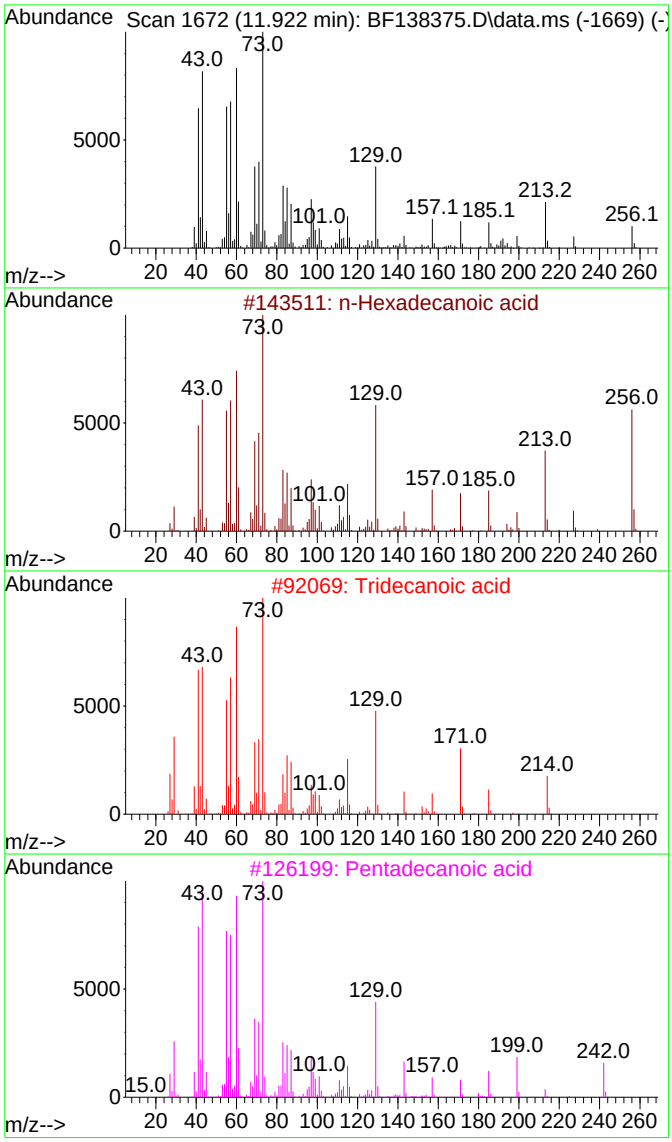
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

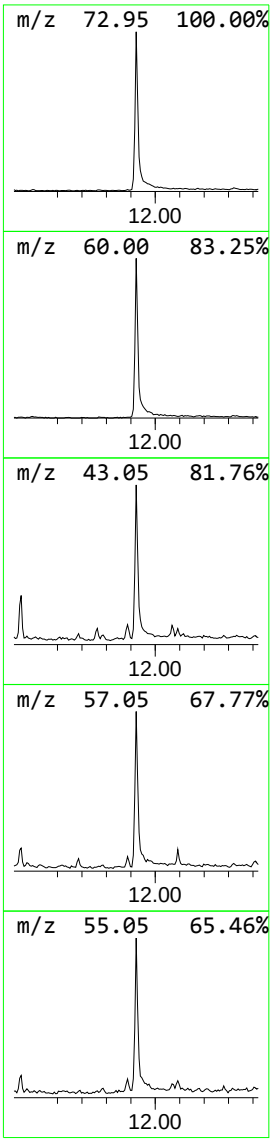
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	11.10 ng	662874	Phenanthrene-d10	11.398

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	92
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138375.D
Acq On : 27 Jun 2024 19:39
Operator : CG\JU
Sample : P3053-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

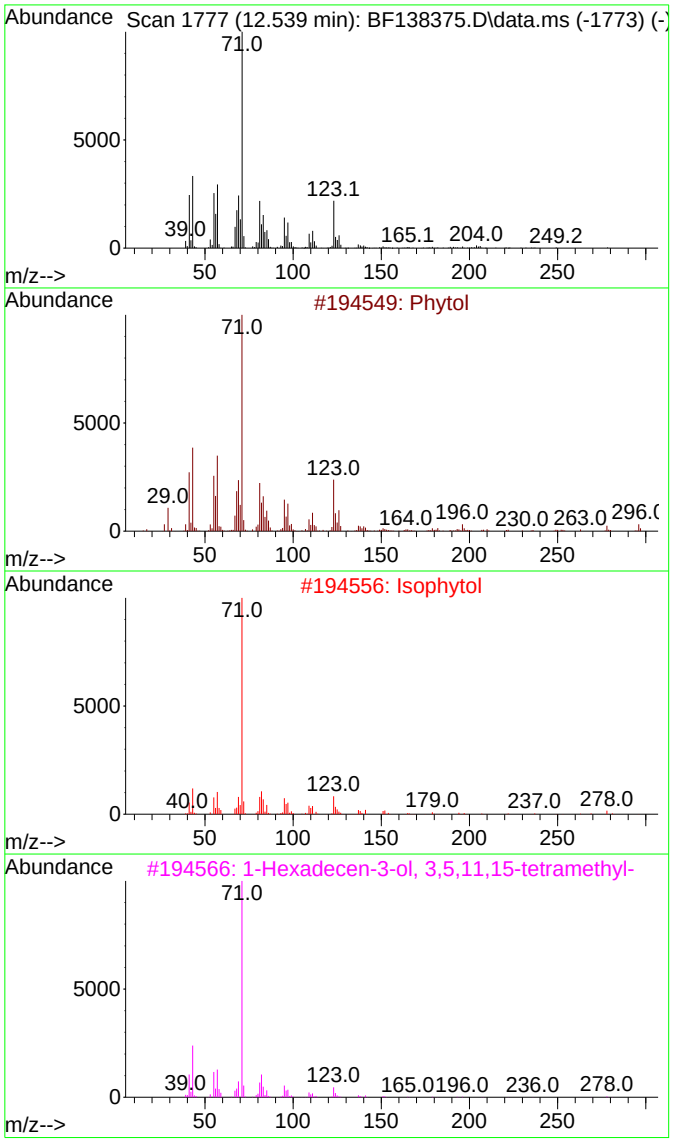
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

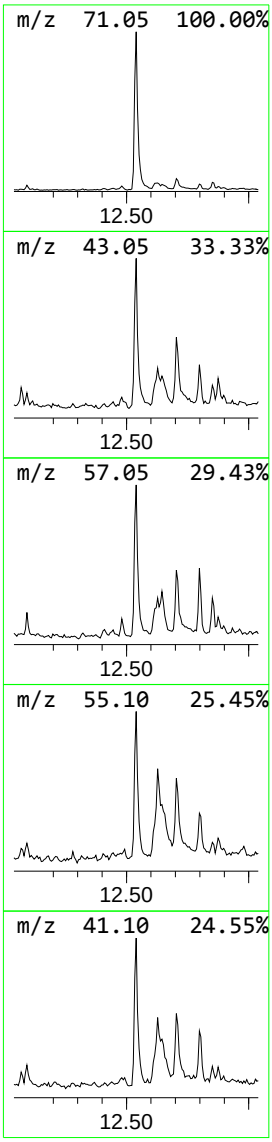
****

Peak Number 5 Phytol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.539	8.12 ng	484951	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phytol	296	C20H40O	000150-86-7	91
2	Isophytol	296	C20H40O	000505-32-8	72
3	1-Hexadecen-3-ol, 3,5,11,15-tetr...	296	C20H40O	1000262-55-5	64
4	Butyric acid, 2-pentadecyl ester	298	C19H38O2	107853-73-6	52
5	Butyric acid, 3-pentadecyl ester	298	C19H38O2	1000280-57-3	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138375.D
Acq On : 27 Jun 2024 19:39
Operator : CG\JU
Sample : P3053-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

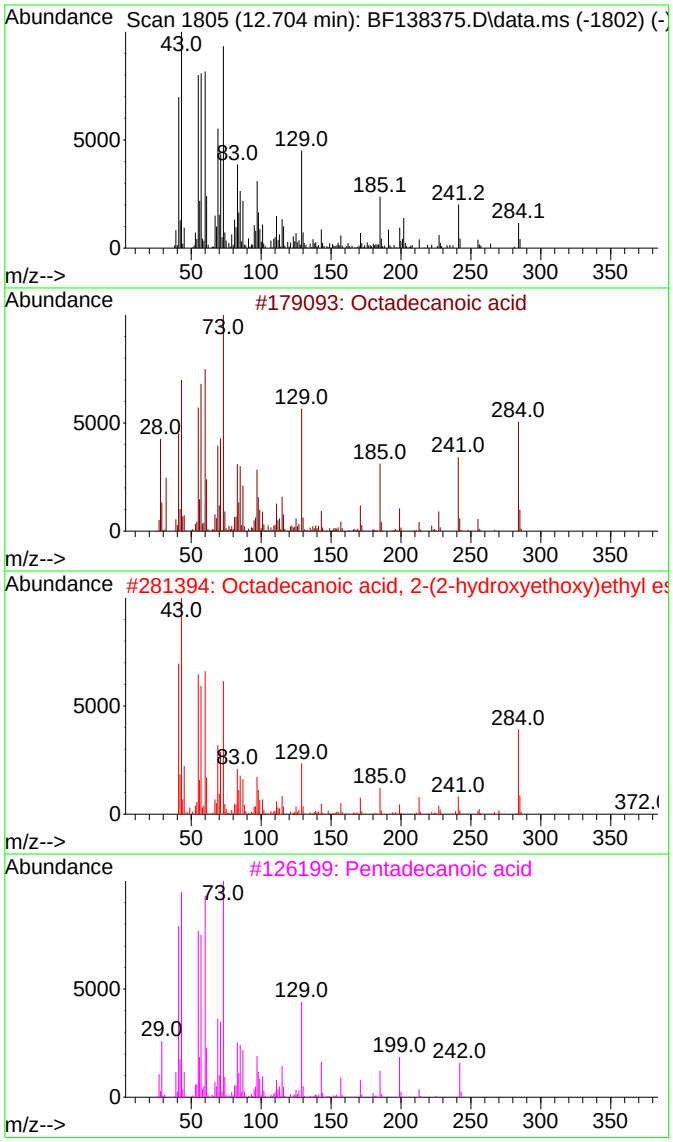
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

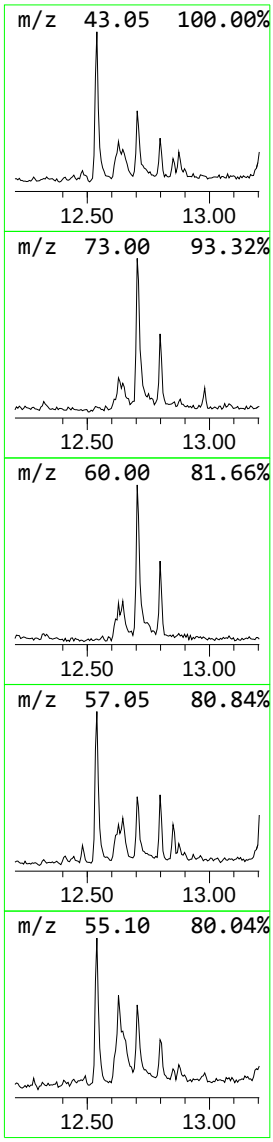
****

Peak Number 6 Octadecanoic acid Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	3.34 ng	199186	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	62





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Operator : CG\JU
Sample : P3053-01
Misc :
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ClientSampleId :
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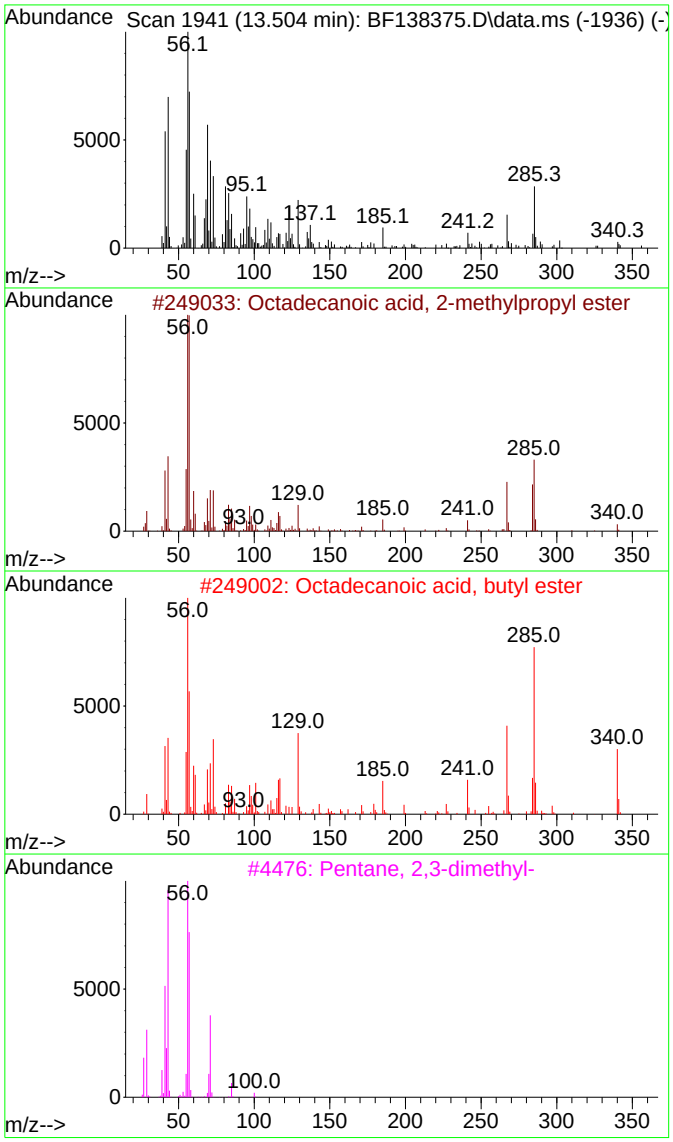
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

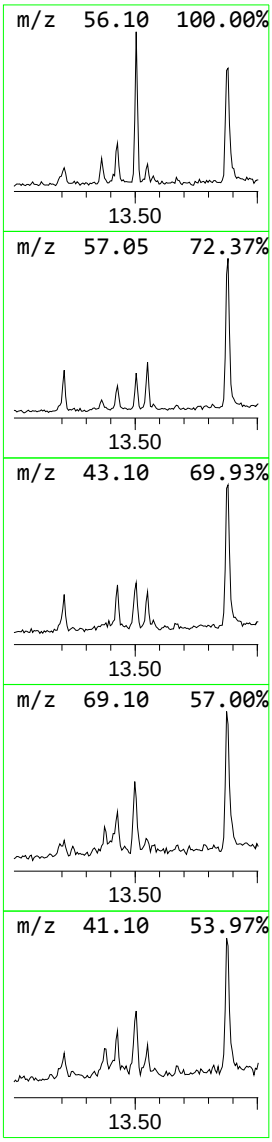
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Octadecanoic acid, 2-methyl... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.504	2.92 ng	202427	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	70
2	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	59
3	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	43
4	Heptane, 2,2,4-trimethyl-	142	C10H22	014720-74-2	38
5	Nipecotic acid	129	C6H11NO2	000498-95-3	38





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ClientSampleId :
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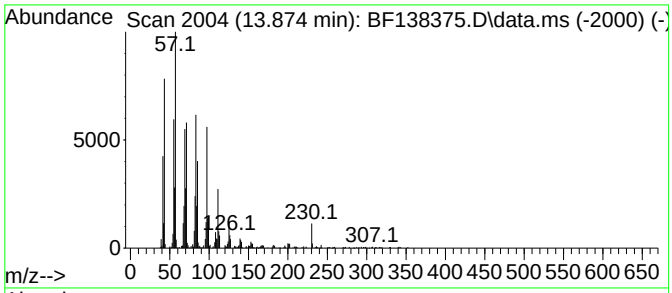
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

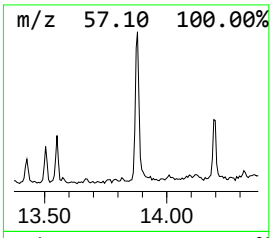
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

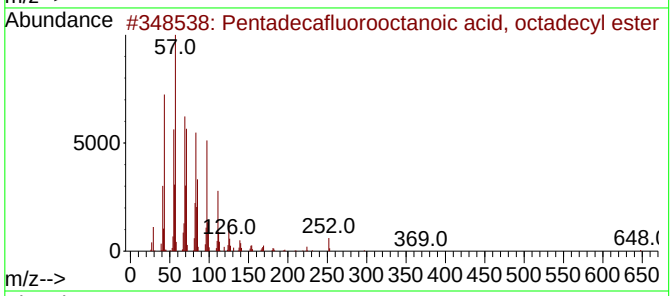
****
Peak Number 8 Pentadecafluorooctanoic aci... Concentration Rank 14

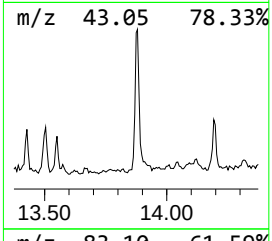
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	7.22 ng	500888	Chrysene-d12	14.033

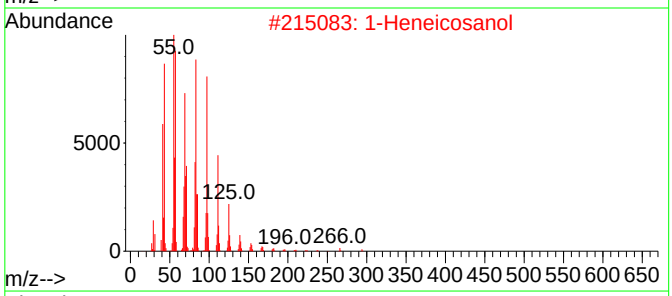
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	92
3	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	90
4	Decane, 5-cyclohexyl-	224	C16H32	013151-76-3	86
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	81

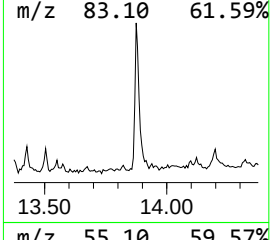


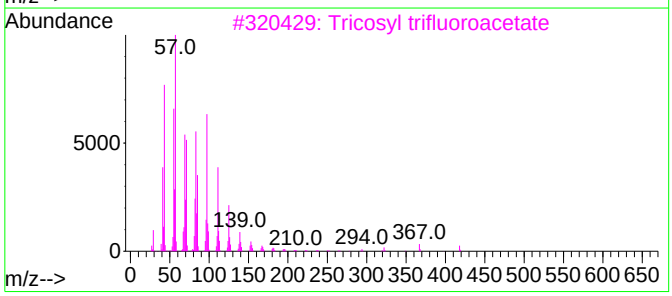


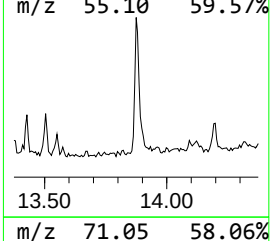


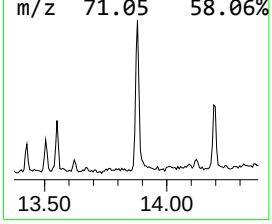












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Acq On : 27 Jun 2024 19:39
Operator : CG\JU
Sample : P3053-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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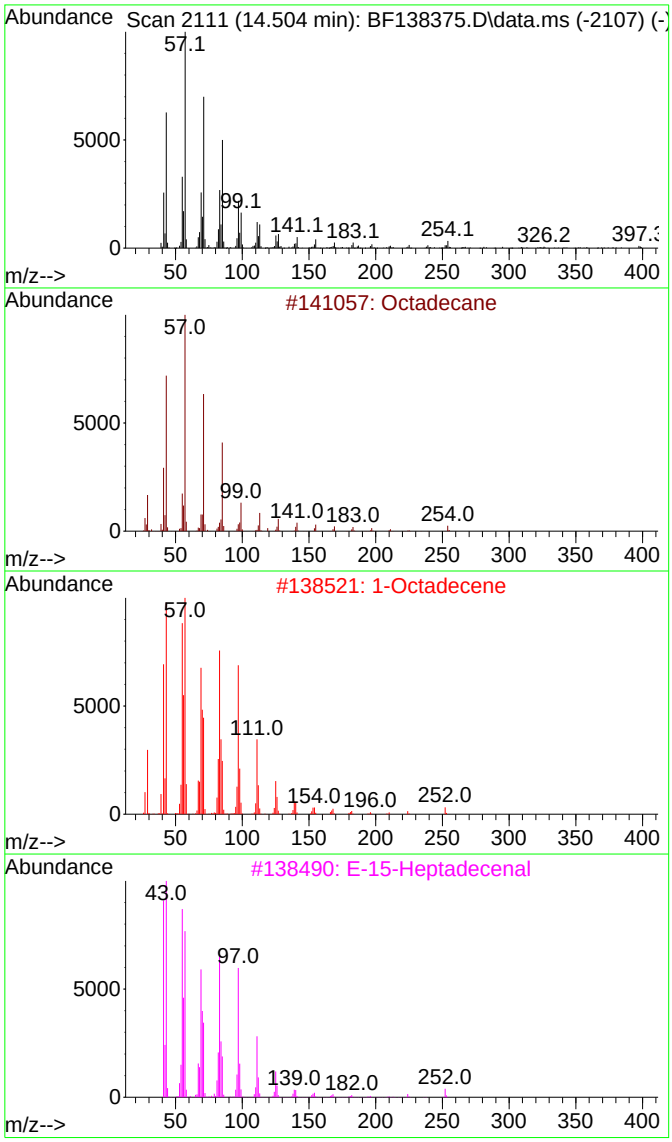
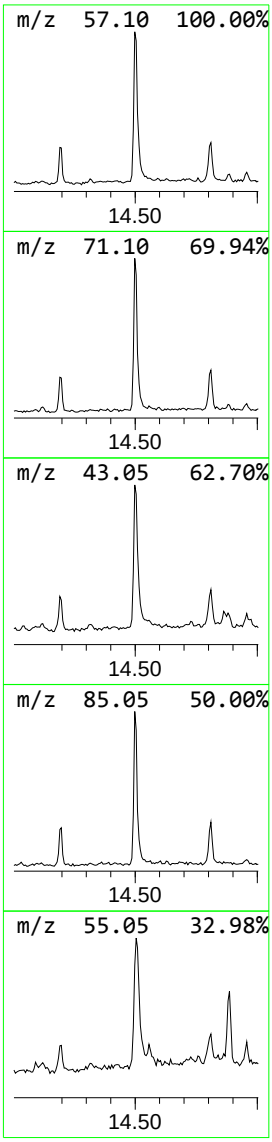
Peak Number 9 Octadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.504	9.49 ng	658641	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	98
2	1-Octadecene	252	C18H36	000112-88-9	95
3	E-15-Heptadecenal	252	C17H32O	1000130-97-9	94
4	1-Heptadecene	238	C17H34	006765-39-5	93
5	Tricosane	324	C23H48	000638-67-5	92





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Sample : P3053-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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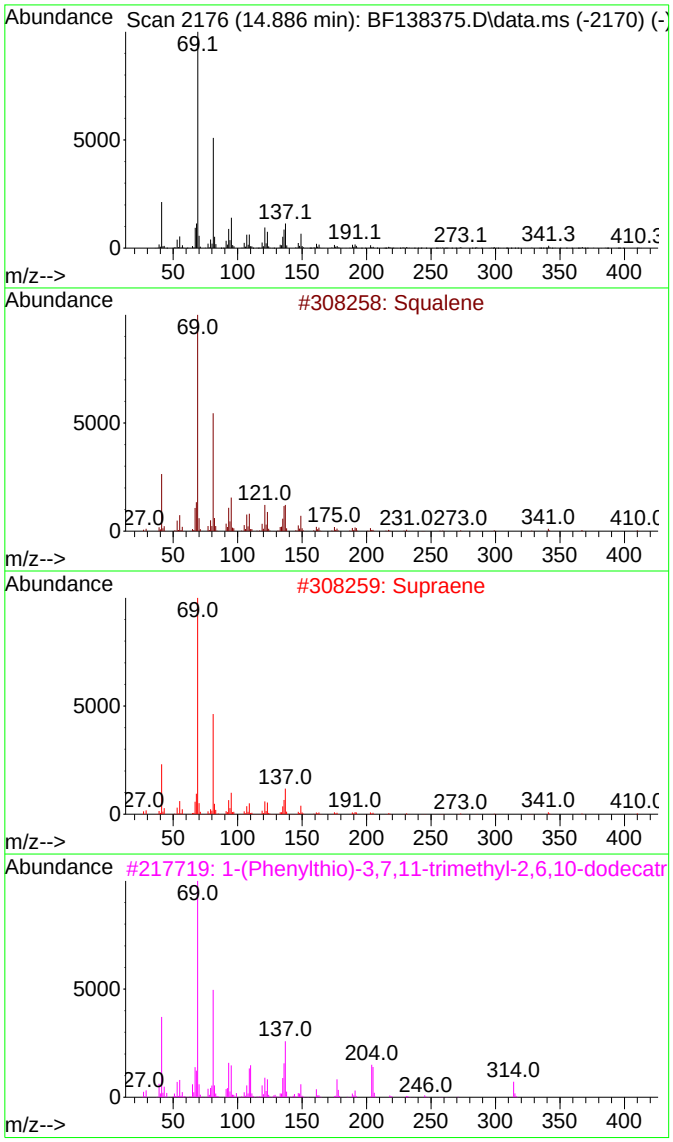
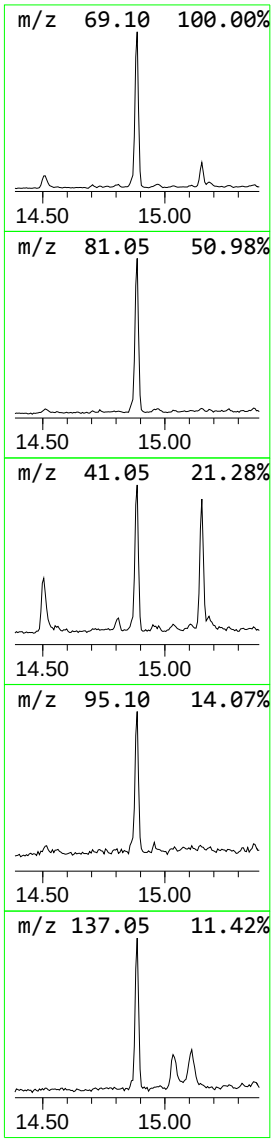
Peak Number 10 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.886	18.14 ng	877089	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	94
2	Supraene	410	C30H50	007683-64-9	91
3	1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	83
4	2,6,10,14-Hexadecatetraenoic aci...	318	C21H34O2	042207-88-5	72
5	3,7,11-Tridecatrienoic acid, 4,8...	264	C17H28O2	036237-70-4	72





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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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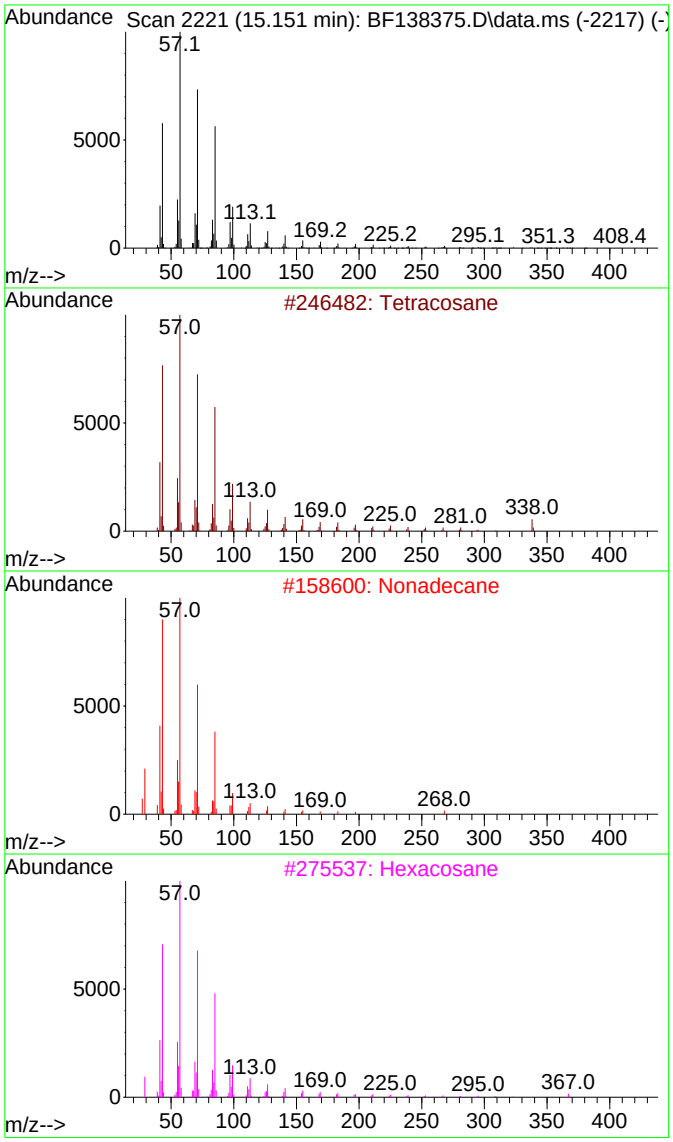
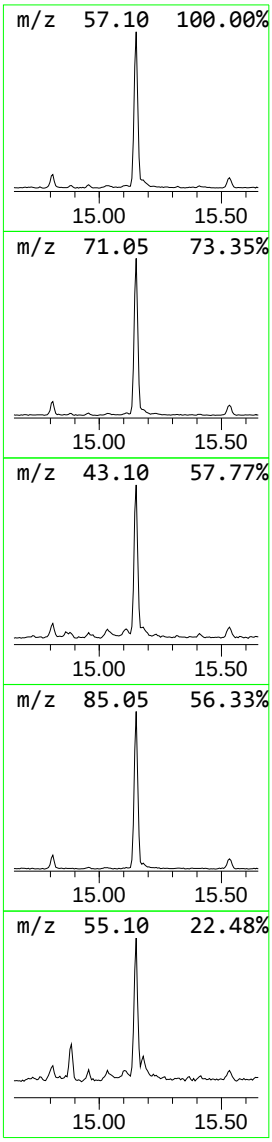
Peak Number 11 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.151	24.20 ng	1170370	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	97
2	Nonadecane	268	C19H40	000629-92-5	95
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91





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ALS Vial : 15 Sample Multiplier: 1

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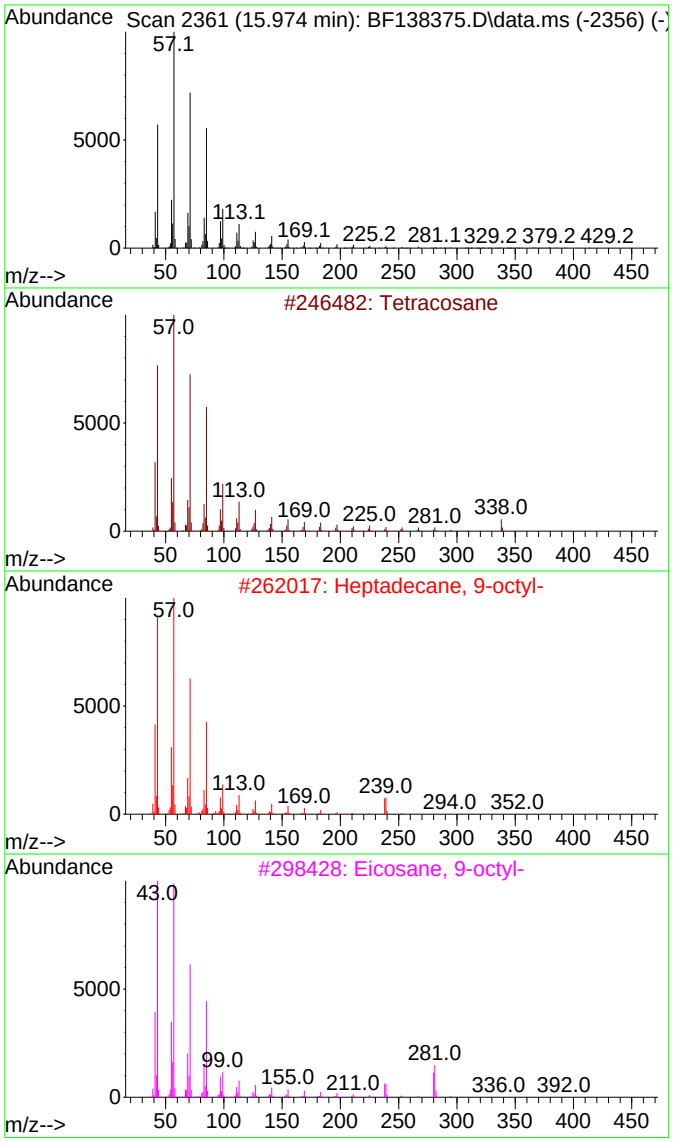
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

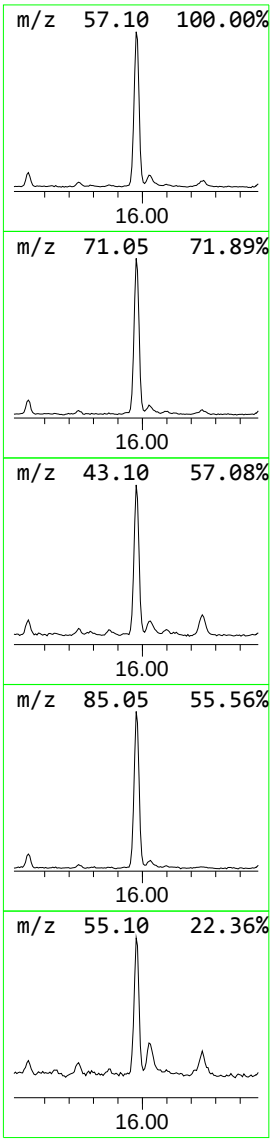
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Heptadecane, 9-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.974	24.45 ng	1182570	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	98
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
3	Eicosane, 9-octyl-	394	C28H58	013475-77-9	94
4	Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	94
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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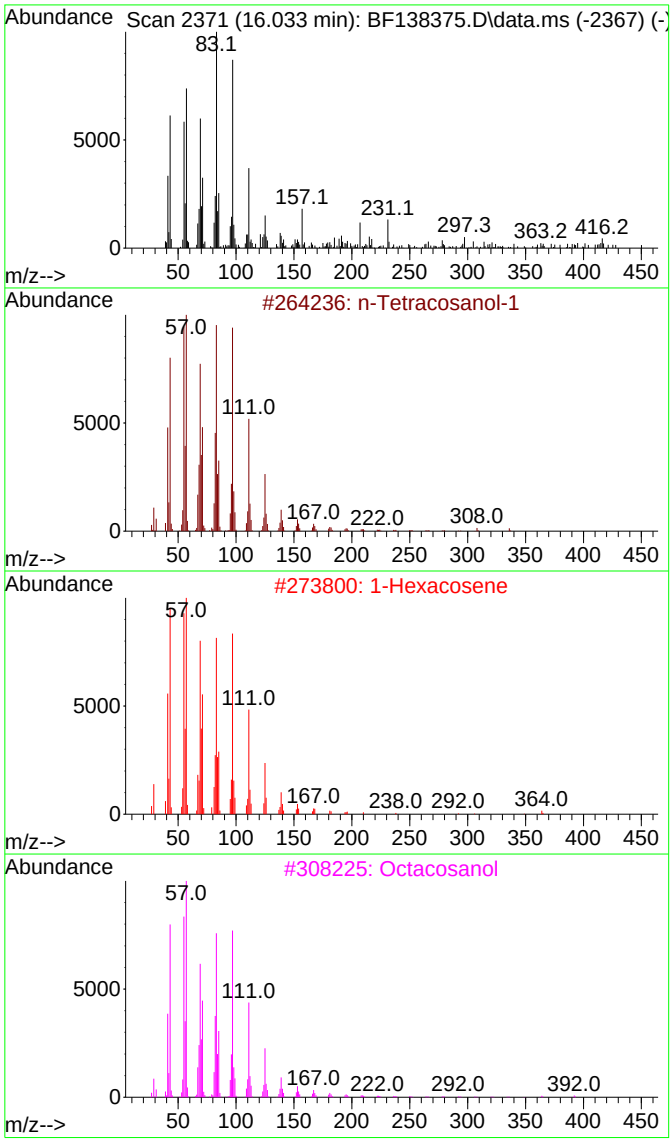
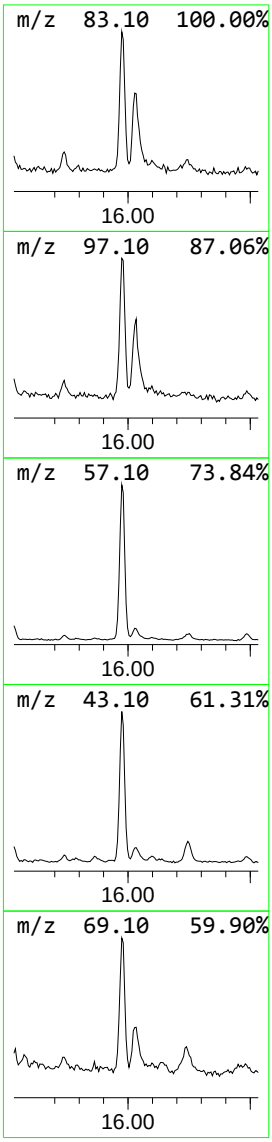
Peak Number 13 n-Tetracosanol-1 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.033	4.36 ng	210840	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	70
2	1-Hexacosene	364	C26H52	018835-33-1	64
3	Octacosanol	410	C28H58O	000557-61-9	55
4	Heptacosyl acetate	438	C29H58O2	1000351-78-2	55
5	Behenic alcohol	326	C22H46O	000661-19-8	50





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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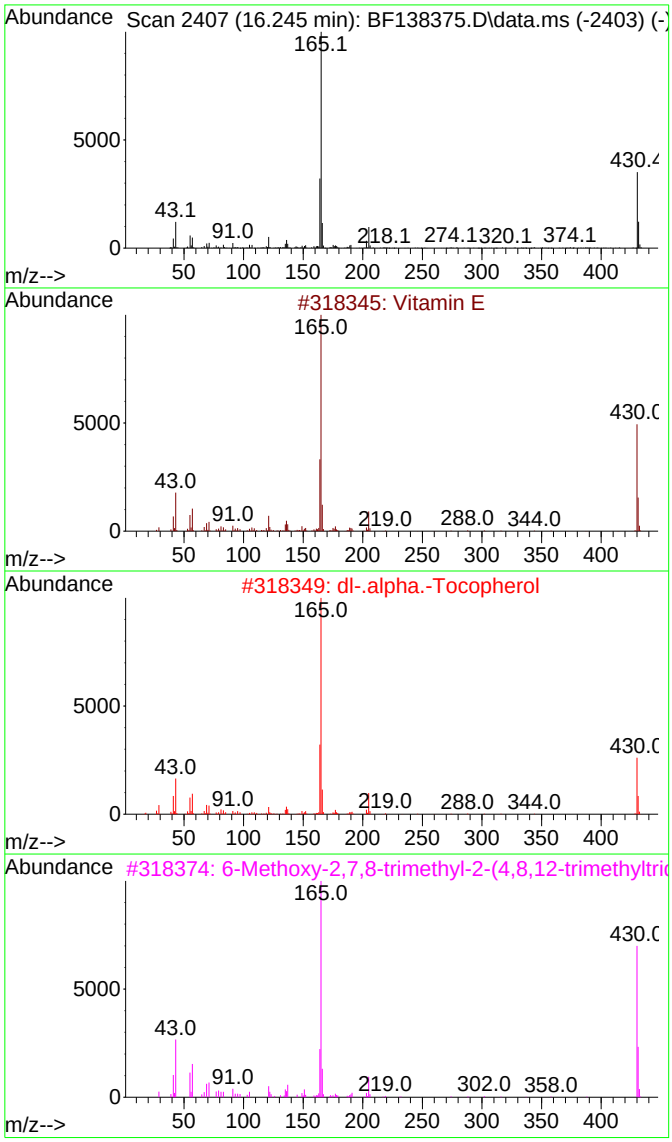
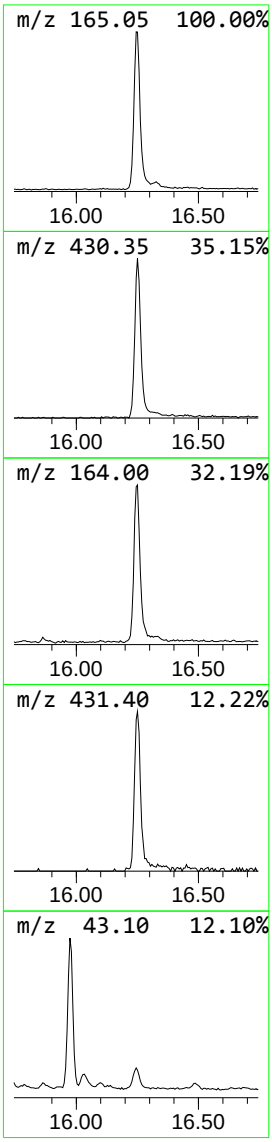
Peak Number 14 Vitamin E Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.245	12.84 ng	620861	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Vitamin E	430	C29H50O2	000059-02-9	94
2	dl-.alpha.-Tocopherol	430	C29H50O2	010191-41-0	94
3	6-Methoxy-2,7,8-trimethyl-2-(4,8...	430	C29H50O2	079306-82-4	93
4	.alpha.-Tocopherol-.beta.-D-mann...	592	C35H60O7	1010156-68-2	83
5	4-Amino-3-methoxypyrazolo[3,4-d]...	165	C6H7N5O	111375-22-5	50





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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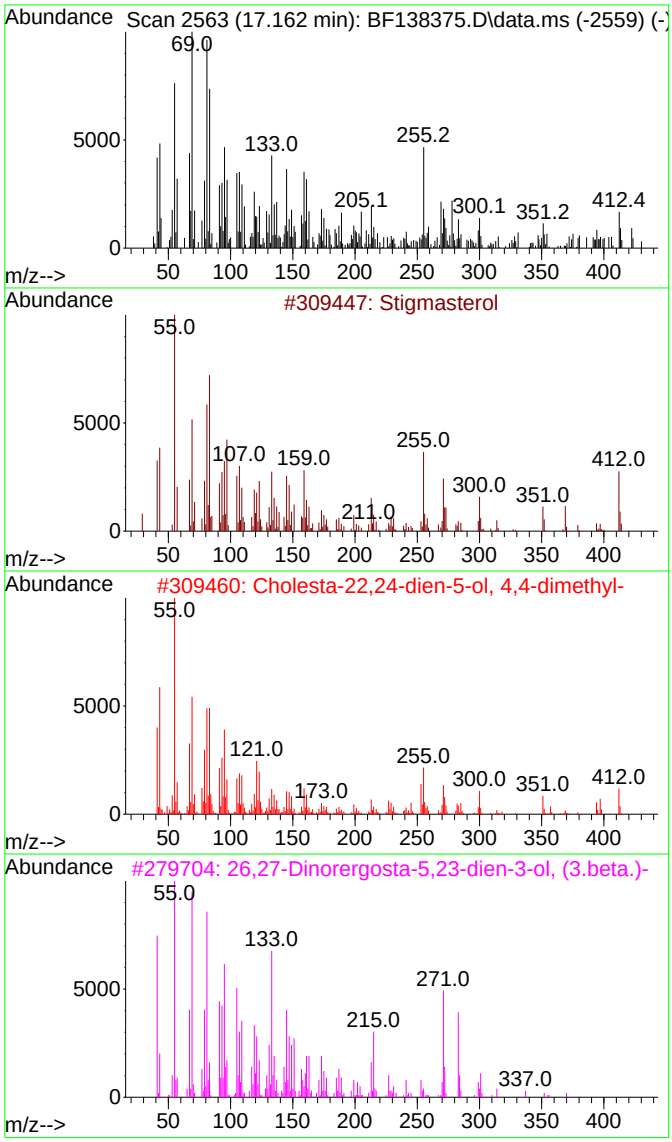
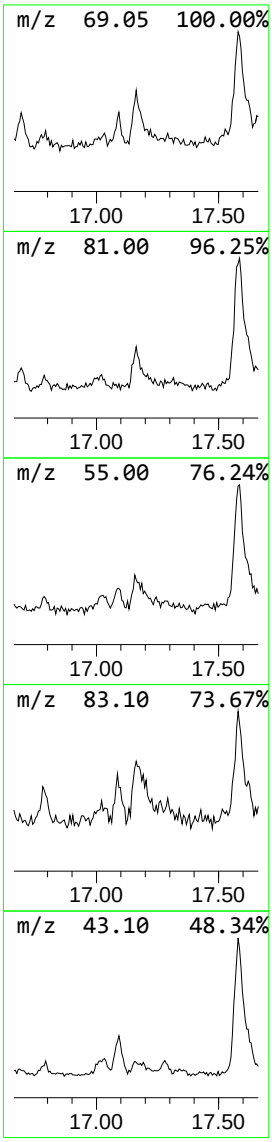
Peak Number 15 Stigmasterol Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.162	4.73 ng	228923	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Stigmasterol	412	C29H48O	000083-48-7	90
2	Cholesta-22,24-dien-5-ol, 4,4-di...	412	C29H48O	1000128-66-1	55
3	26,27-Dinorergosta-5,23-dien-3-o...	370	C26H42O	035882-88-3	41
4	Stigmastan-6,22-dien, 3,5-dedihy...	394	C29H46	107304-12-1	27
5	Methyl (3S,4aR)-1-(furan-2-ylmet...	412	C23H28N2O5	1000464-93-8	25





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TIC Library : C:\Database\NIST20.L
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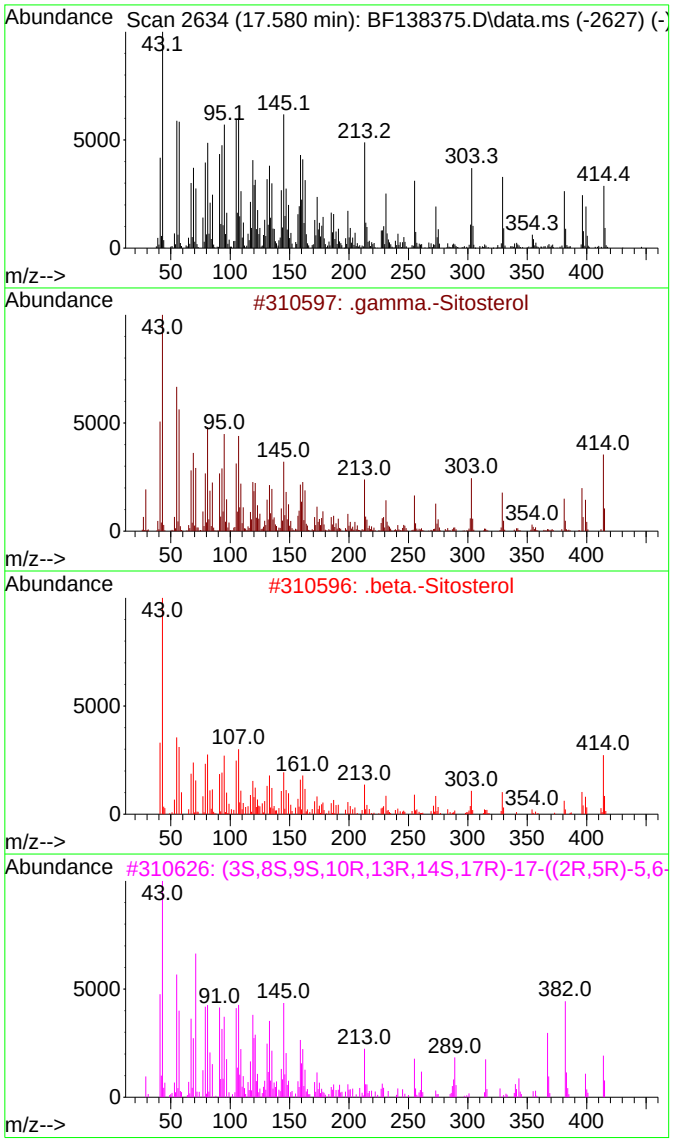
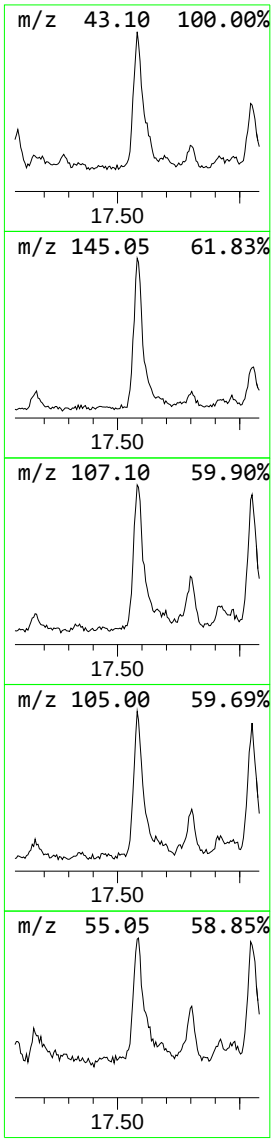
Peak Number 16 .gamma.-Sitosterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.580	41.57 ng	2010240	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	94
3	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	48
4	(3S,8S,9S,10R,13R,14S,17R)-17-((...	428	C30H52O	020194-50-7	22
5	Campesterol	400	C28H48O	000474-62-4	15





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Data File : BF138375.D
Acq On : 27 Jun 2024 19:39
Operator : CG\JU
Sample : P3053-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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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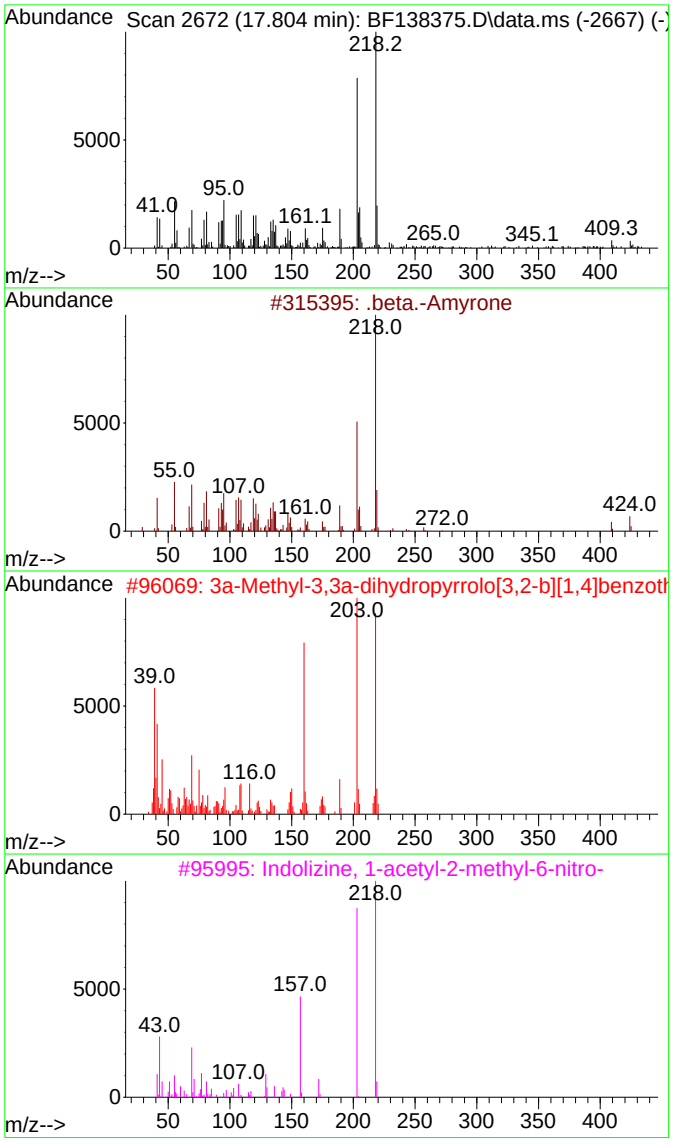
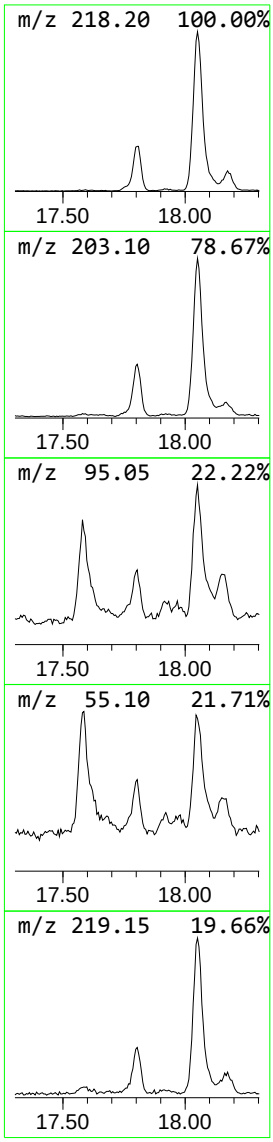
Peak Number 17 .beta.-Amyrone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.804	12.01 ng	580660	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Amyrone	424	C30H48O	000638-97-1	68
2	3a-Methyl-3,3a-dihydropyrrolo[3,...	218	C11H10N2OS	017163-68-7	64
3	Indolizine, 1-acetyl-2-methyl-6-...	218	C11H10N2O3	1000071-33-1	64
4	Olean-12-en-3-ol, acetate, (3.be...	468	C32H52O2	001616-93-9	62
5	2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	58





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Data File : BF138375.D
Acq On : 27 Jun 2024 19:39
Operator : CG\JU
Sample : P3053-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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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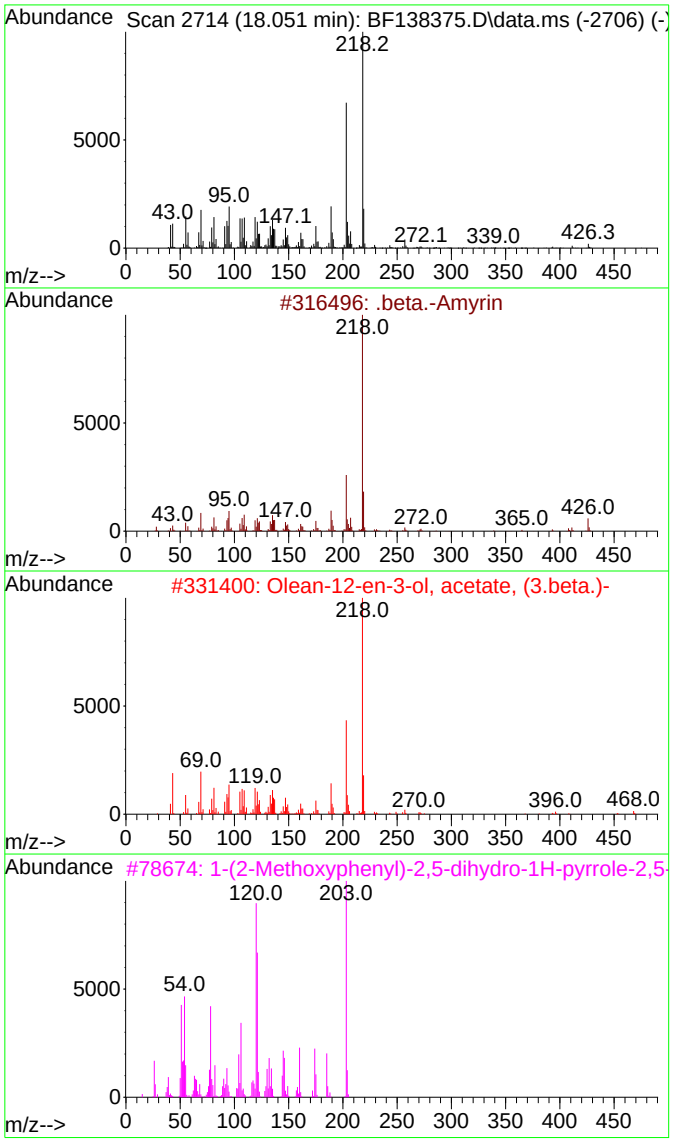
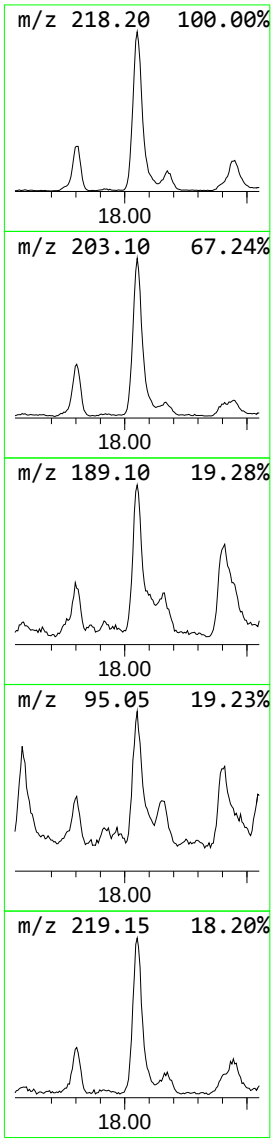
Peak Number 18 .beta.-Amyrin Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.051	45.86 ng	2217570	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Amyrin	426	C30H50O	000559-70-6	97
2	Olean-12-en-3-ol, acetate, (3.be...	468	C32H52O2	001616-93-9	91
3	1-(2-Methoxyphenyl)-2,5-dihydro-...	203	C11H9NO3	017392-68-6	91
4	2H-Cyclopropa[a]naphthalen-2-one...	218	C15H22O	006831-17-0	89
5	.beta.-Amyrone	424	C30H48O	000638-97-1	87





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Data File : BF138375.D
Acq On : 27 Jun 2024 19:39
Operator : CG\JU
Sample : P3053-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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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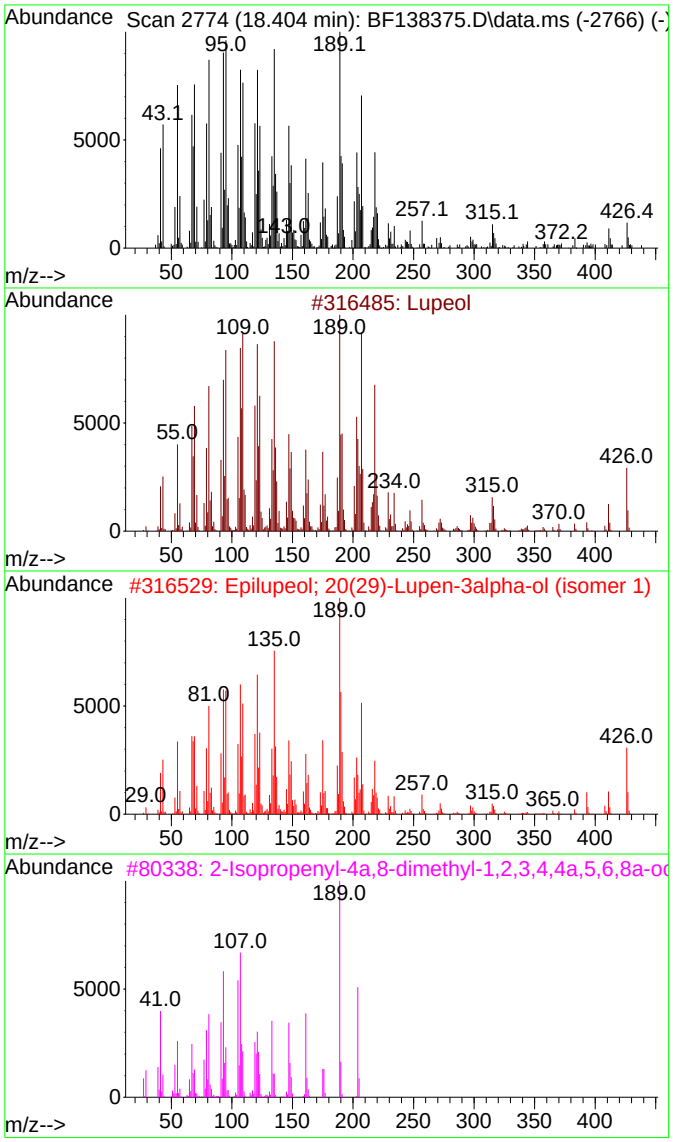
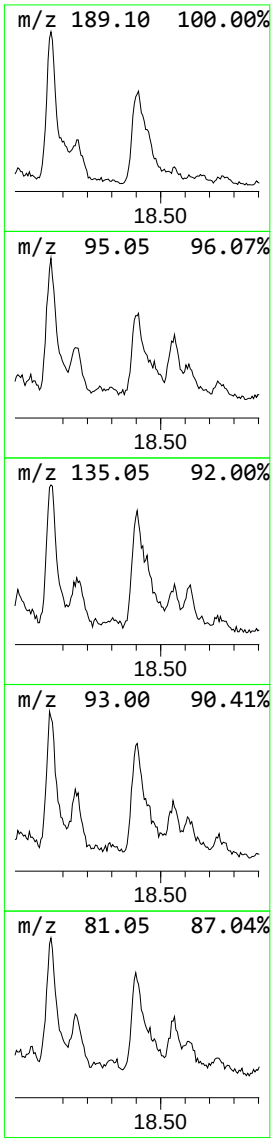
Peak Number 19 Lupeol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.404	36.11 ng	1746240	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lupeol	426	C30H50O	000545-47-1	99
2	Epilupeol; 20(29)-Lupen-3alpha-o...	426	C30H50O	1000513-01-3	90
3	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	207297-57-2	78
4	Lupeol, trifluoroacetate	522	C32H49F3O2	1000394-56-7	70
5	Germanicol	426	C30H50O	000465-02-1	70





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Data File : BF138375.D
Acq On : 27 Jun 2024 19:39
Operator : CG\JU
Sample : P3053-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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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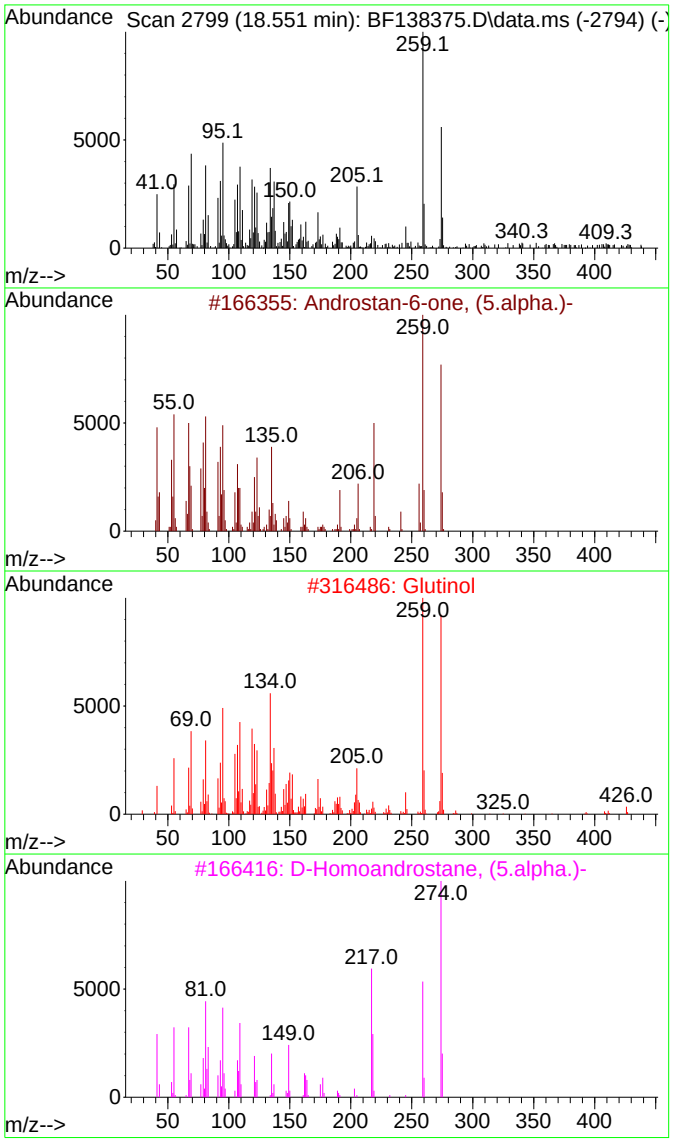
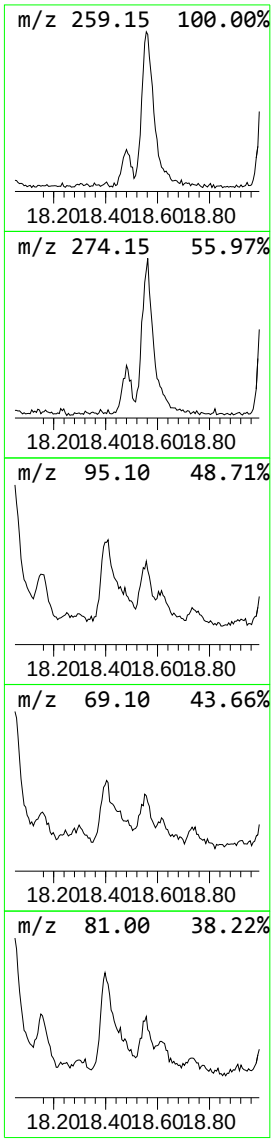
Peak Number 20 Androstan-6-one, (5.alpha.)- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.551	7.27 ng	351718	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Androstan-6-one, (5.alpha.)-	274	C19H30O	003676-06-0	58
2	Glutinol	426	C30H50O	000545-24-4	46
3	D-Homoandrostane, (5.alpha.)-	274	C20H34	035575-26-9	38
4	3-Methyl-3-(naphthalen-1-yl)isob...	274	C19H14O2	078772-71-1	35
5	Pyridine, 3,5-di(4-methylphenyl)-	259	C19H17N	1000380-54-8	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138375.D
Acq On : 27 Jun 2024 19:39
Operator : CG\JU
Sample : P3053-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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
Butane, 2-metho...	2.175	39.8	ng	2595900	1	6.881	1306230	20.0
2-Pentanone, 4-...	5.098	3.9	ng	253241	1	6.881	1306230	20.0
1-Phenoxypropan...	8.469	3.3	ng	264289	2	8.157	1582980	20.0
n-Hexadecanoic ...	11.922	11.1	ng	662874	4	11.398	1193940	20.0
Phytol	12.539	8.1	ng	484951	4	11.398	1193940	20.0
Octadecanoic acid	12.704	3.3	ng	199186	4	11.398	1193940	20.0
Octadecanoic ac...	13.504	2.9	ng	202427	5	14.033	1387460	20.0
Pentadecafluoro...	13.874	7.2	ng	500888	5	14.033	1387460	20.0
Octadecane	14.504	9.5	ng	658641	5	14.033	1387460	20.0
Squalene	14.886	18.1	ng	877089	6	15.504	967166	20.0
Tetracosane	15.151	24.2	ng	1170370	6	15.504	967166	20.0
Heptadecane, 9-...	15.974	24.4	ng	1182570	6	15.504	967166	20.0
n-Tetracosanol-1	16.033	4.4	ng	210840	6	15.504	967166	20.0
Vitamin E	16.245	12.8	ng	620861	6	15.504	967166	20.0
Stigmasterol	17.162	4.7	ng	228923	6	15.504	967166	20.0
.gamma.-Sitosterol	17.580	41.6	ng	2010240	6	15.504	967166	20.0
.beta.-Amyrone	17.804	12.0	ng	580660	6	15.504	967166	20.0
.beta.-Amyrin	18.051	45.9	ng	2217570	6	15.504	967166	20.0
Lupeol	18.404	36.1	ng	1746240	6	15.504	967166	20.0
Androstan-6-one...	18.551	7.3	ng	351718	6	15.504	967166	20.0