LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136737.D
Acq On : 27 Dec 2023 00:40
Operator : CG\JU
Sample : 05812-01RE
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW2RE

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136737.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.157	8	12	20	rVB3	8445	13569	1.25%	0.189%
2	2.851	124	130	135	rBV	11762	17896	1.65%	0.249%
3	3.634	257	263	268	rBV2	10177	15328	1.41%	0.213%
4	3.845	296	299	307	rVB	9959	13728	1.27%	0.191%
5	4.998	493	495	500	rVB	21970	22177	2.05%	0.309%
6	5.092	507	511	515	rBV	78221	73091	6.74%	1.018%
7	5.422	563	567	576	rBV	104614	102011	9.41%	1.420%
8	6.428	735	738	745	rBV	83269	86391	7.97%	1.203%
9	6.610	766	769	775	rBV	29509	33830	3.12%	0.471%
10	6.781	795	798	804	rVB	536974	420466	38.80%	5.854%
11	6.851	807	810	812	rBV	16334	15153	1.40%	0.211%
12	7.339	889	893	896	rBV	665329	583858	53.87%	8.129%
13	7.598	932	937	942	rVB	57994	46046	4.25%	0.641%
14	8.057	1011	1015	1019	rBV	650082	526590	48.59%	7.331%
15	8.375	1066	1069	1083	rBV	58456	89514	8.26%	1.246%
16	9.133	1194	1198	1206	rBV	1290062	1083752	100.00%	15.088%
17	9.216	1209	1212	1214	rBV	31218	22076	2.04%	0.307%
18	9.816	1310	1314	1317	rBV	649987	522210	48.19%	7.270%
19	9.916	1326	1331	1338	rBV	105355	143828	13.27%	2.002%
20	10.345	1400	1404	1408	rVB2	19269	17979	1.66%	0.250%
21	10.604	1445	1448	1452	rBV	114941	100416	9.27%	1.398%
22	10.722	1466	1468	1477	rVB3	29397	36094	3.33%	0.503%
23	10.974	1508	1511	1516	rBV6	9937	12533	1.16%	0.174%
24	11.174	1538	1545	1547	rBV	21617	23378	2.16%	0.325%
25	11.204	1547	1550	1557	rVB4	14617	17991	1.66%	0.250%
26	11.304	1564	1567	1570	rBV	497287	444941	41.06%	6.195%
27	11.704	1631	1635	1637	rBV2	20593	19254	1.78%	0.268%
28	11.769	1643	1646	1649	rBV4	8522	12393	1.14%	0.173%
29	11.845	1655	1659	1670	rBV	357485	367605	33.92%	5.118%
30	12.092	1698	1701	1706	rBV2	71646	60447	5.58%	0.842%
31	12.139	1706	1709	1712	rVB2	17651	17764	1.64%	0.247%
32	12.416	1751	1756	1760	rBV6	11956	19942	1.84%	0.278%
33	12.521	1772	1774	1777	rBV	17580	18199	1.68%	0.253%
34	12.568	1777	1782	1788	rVB6	18301	33026	3.05%	0.460%
35	12.627	1790	1792	1803	rBV2	70671	89852	8.29%	1.251%
36	12.721	1806	1808	1811	rBV3	21585	19670	1.81%	0.274%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136737.D
Acq On : 27 Dec 2023 00:40
Operator : CG\JU
Sample : 05812-01RE
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW2RE

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.751	1811	1813	1816	rVB	16571	14059	1.30%	0.196%
38	12.898	1834	1838	1842	rBV	670330	586567	54.12%	8.166%
39	13.133	1876	1878	1881	rBV	13219	13070	1.21%	0.182%
40	13.480	1932	1937	1939	rBV3	22052	29897	2.76%	0.416%
41	13.839	1991	1998	2011	rBV6	115430	360381	33.25%	5.017%
42	13.962	2014	2019	2022	rVV	446517	435845	40.22%	6.068%
43	14.110	2041	2044	2046	rBV	46385	45902	4.24%	0.639%
44	14.439	2097	2100	2103	rVB	23324	21430	1.98%	0.298%
45	14.598	2124	2127	2131	rVB	37808	41552	3.83%	0.578%
46	14.821	2161	2165	2169	rBV	100442	112060	10.34%	1.560%
47	15.086	2208	2210	2214	rVB2	28705	30626	2.83%	0.426%
48	15.439	2265	2270	2274	rBV	278679	348444	32.15%	4.851%

Sum of corrected areas: 7182831

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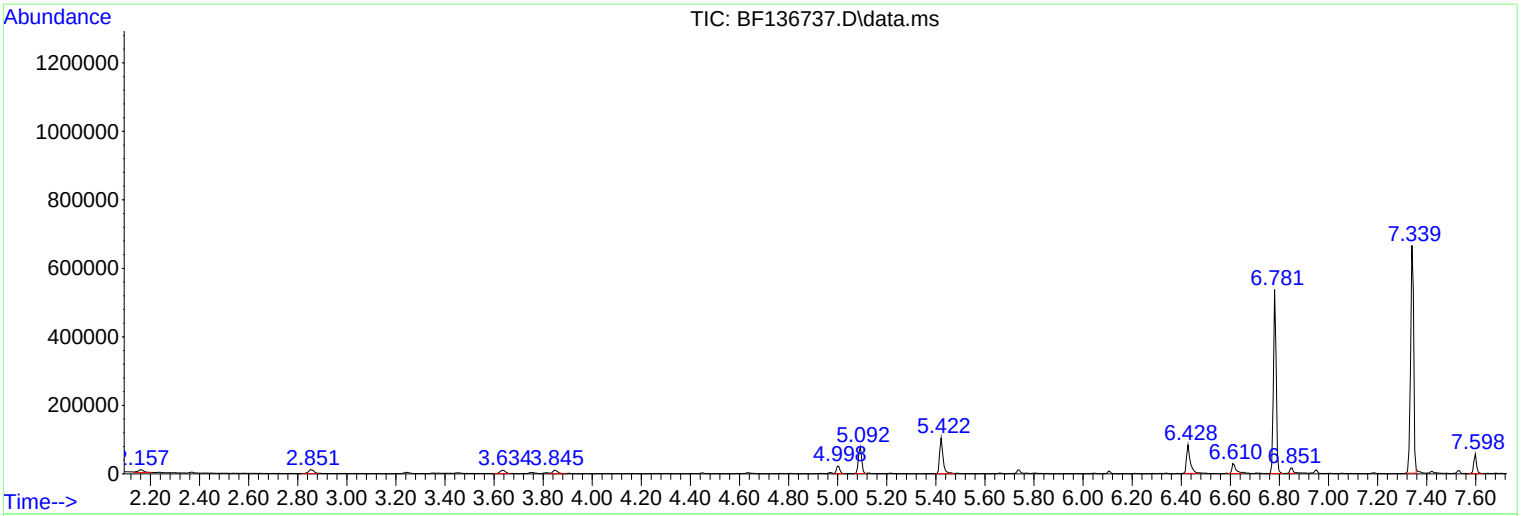
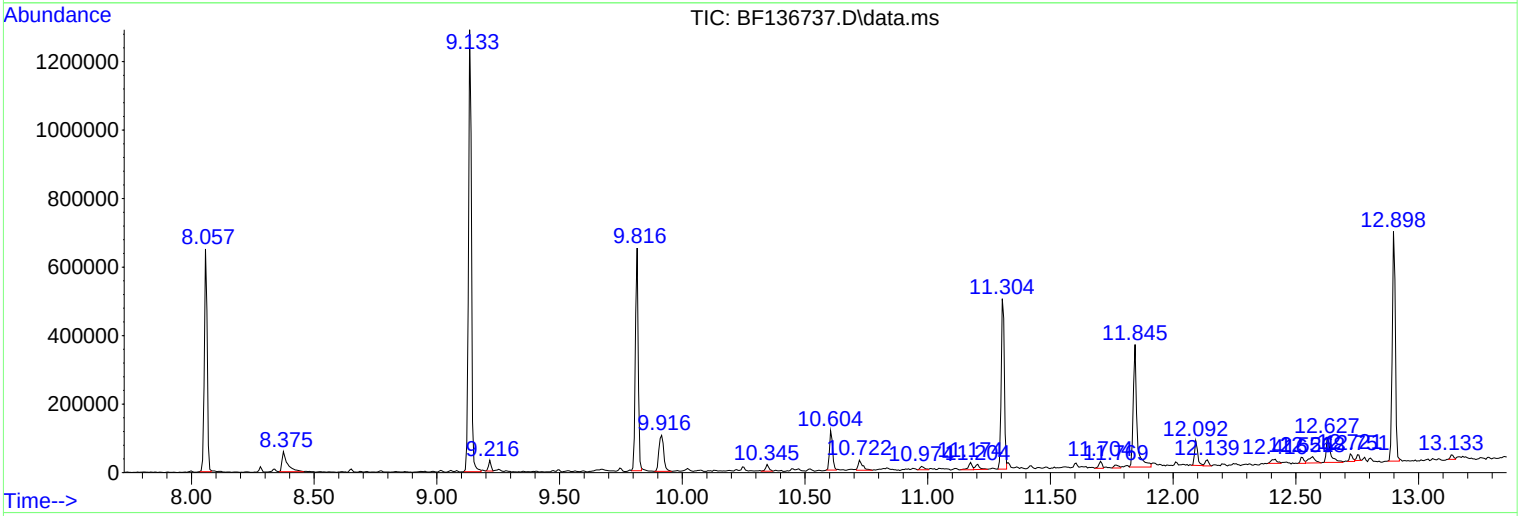
Misc :
ALS Vial : 14 Sample Multiplier: 1

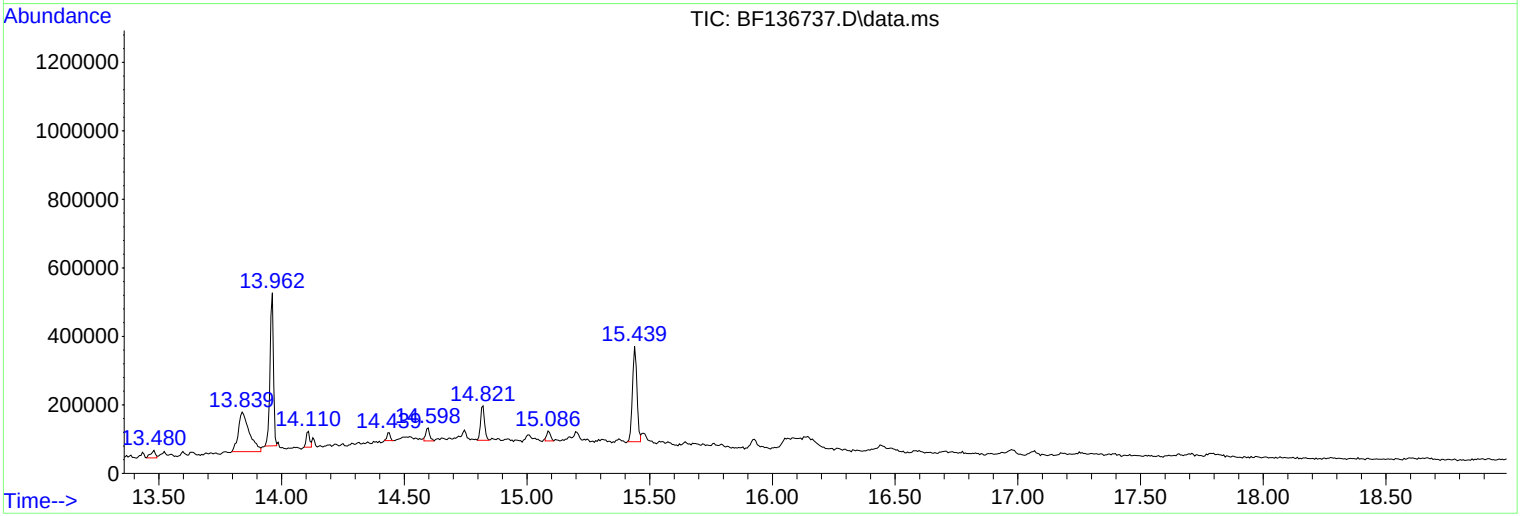
Instrument :
BNA_F
ClientSampleId :
RW2RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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\BF122623\
Data File : BF136737.D
Acq On : 27 Dec 2023 00:40
Operator : CG\JU
Sample : 05812-01RE
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW2RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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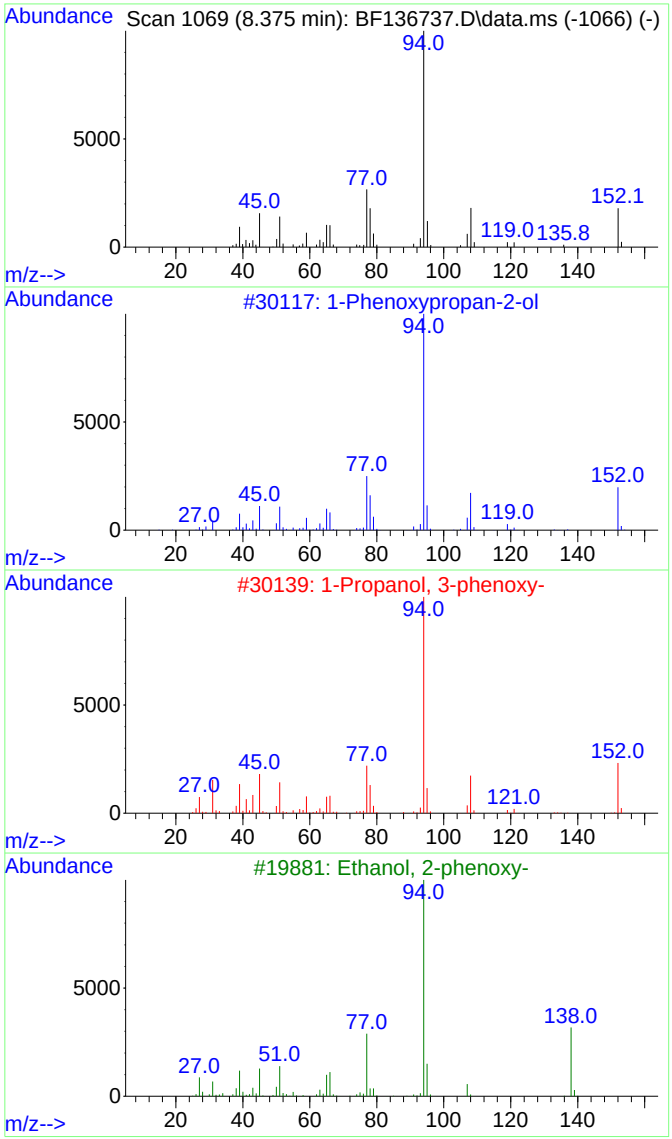
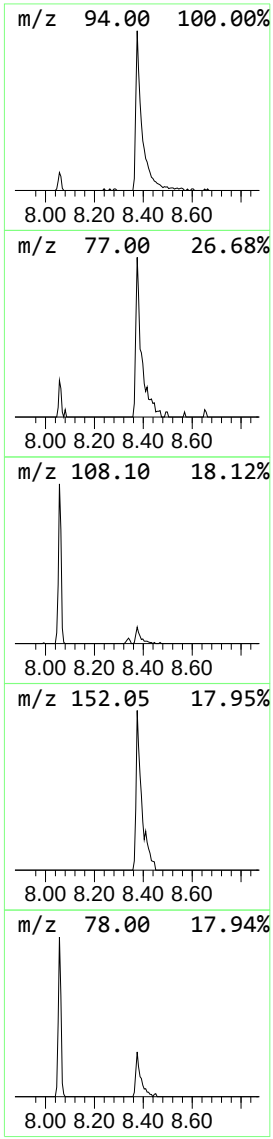
Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.375	3.40 ng	89514	Naphthalene-d8	8.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	97
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	94
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136737.D
Acq On : 27 Dec 2023 00:40
Operator : CG\JU
Sample : 05812-01RE
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW2RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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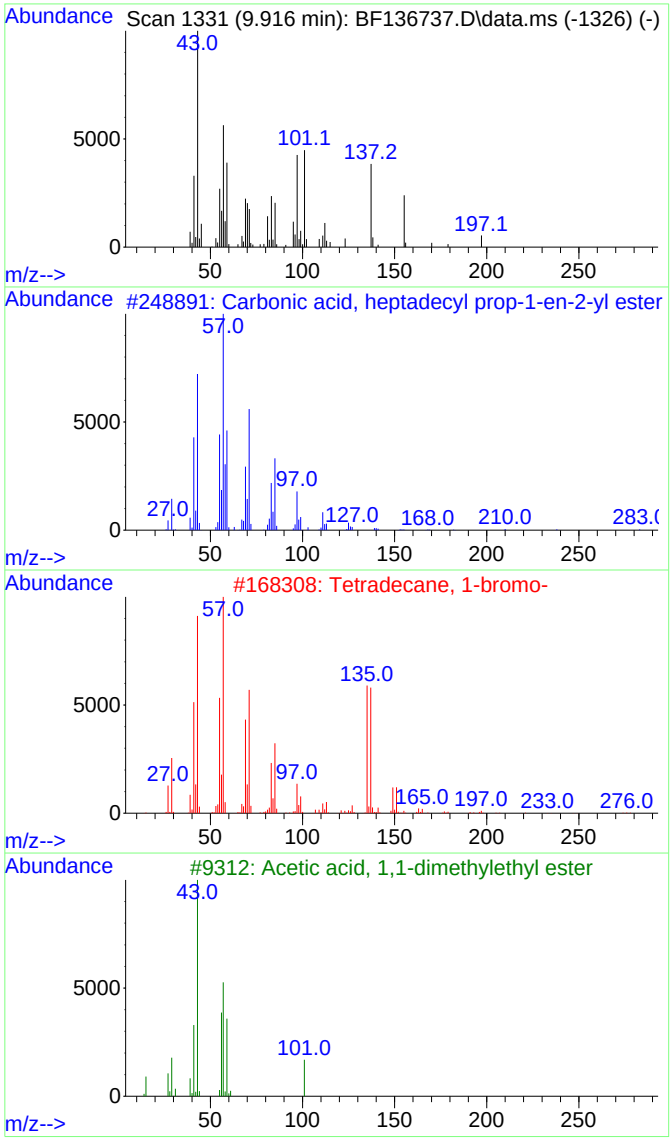
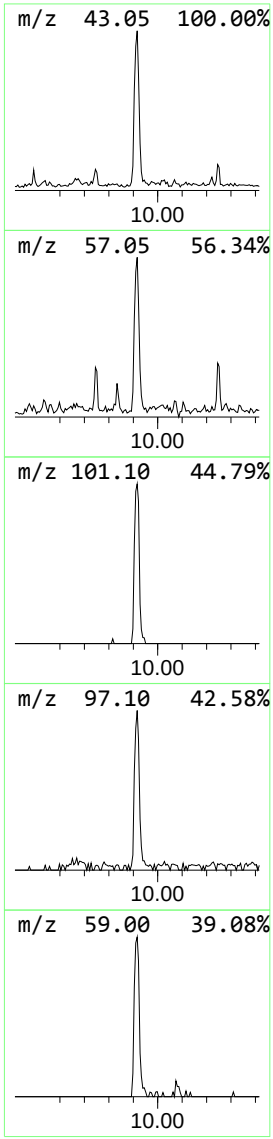
Peak Number 3 unknown9.916 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.916	5.51 ng	143828	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, heptadecyl prop-1...	340	C21H40O3	1000382-90-2	25
2	Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	14
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	14
4	Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	10
5	6,10,13-Trimethyltetradecanol	256	C17H36O	1000131-71-0	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136737.D
Acq On : 27 Dec 2023 00:40
Operator : CG\JU
Sample : 05812-01RE
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW2RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

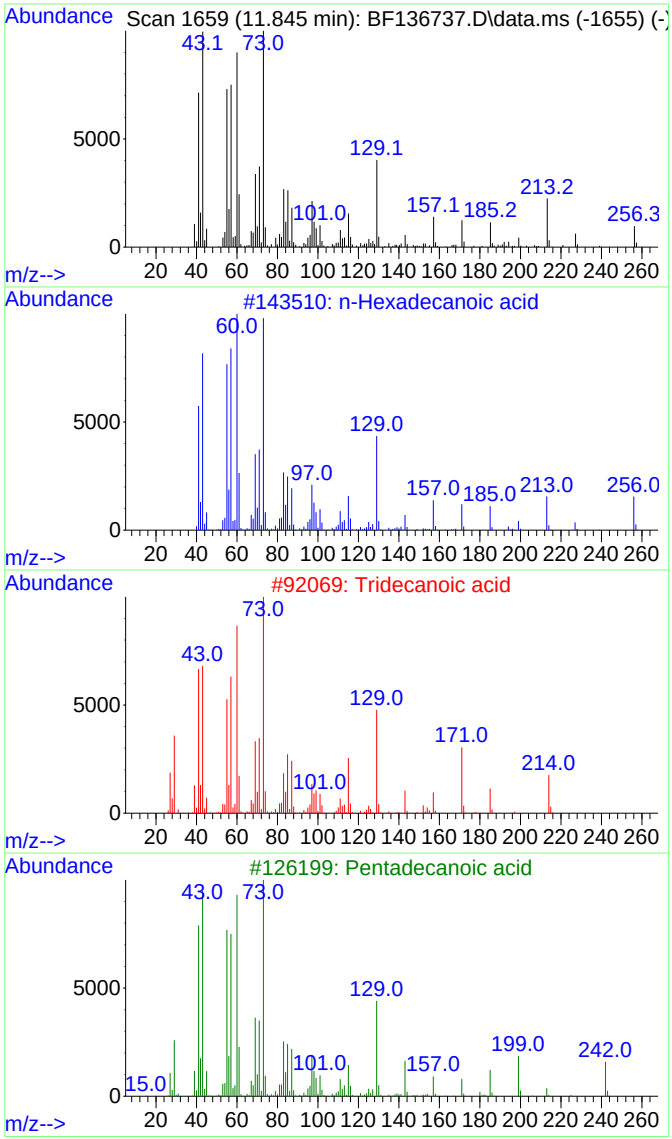
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

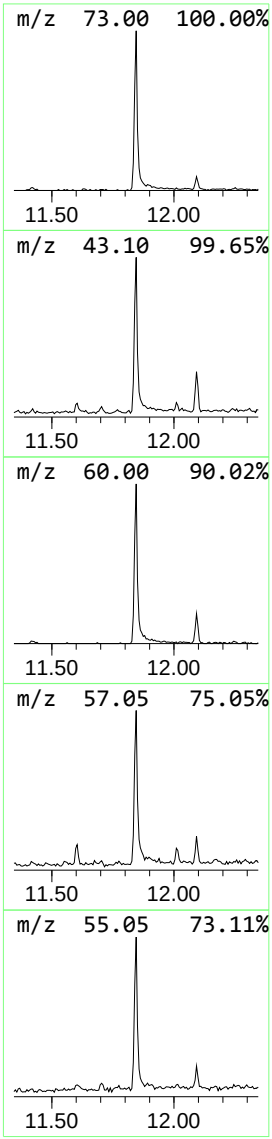
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	16.52 ng	367605	Phenanthrene-d10	11.304

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	96
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5	Undecanoic acid	186	C11H22O2	000112-37-8	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136737.D
Acq On : 27 Dec 2023 00:40
Operator : CG\JU
Sample : 05812-01RE
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW2RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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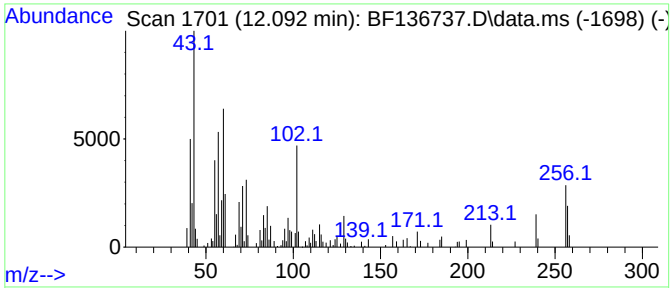
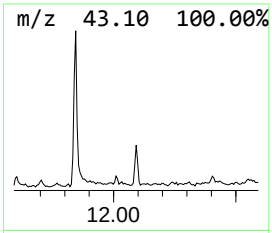
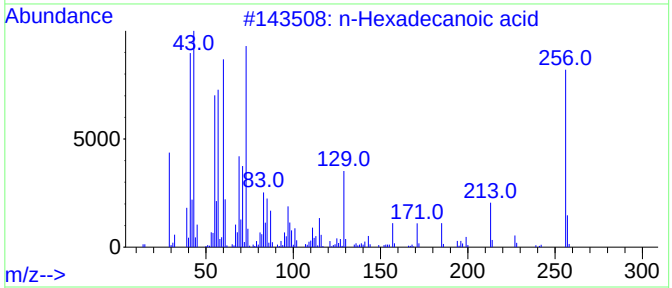
Peak Number 5 Isopropyl palmitate Concentration Rank 8

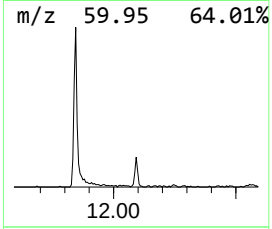
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.092	2.72 ng	60447	Phenanthrene-d10	11.304

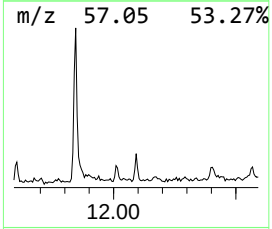
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
2	Isopropyl palmitate	298	C19H38O2	000142-91-6	59
3	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	52
4	Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	49
5	i-Propyl 14-methyl-pentadecanoate	298	C19H38O2	1000336-62-4	38

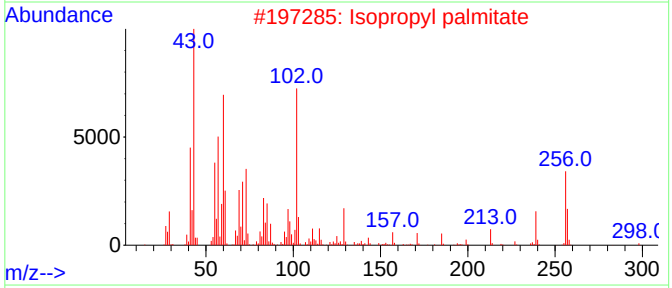


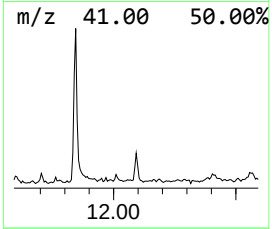


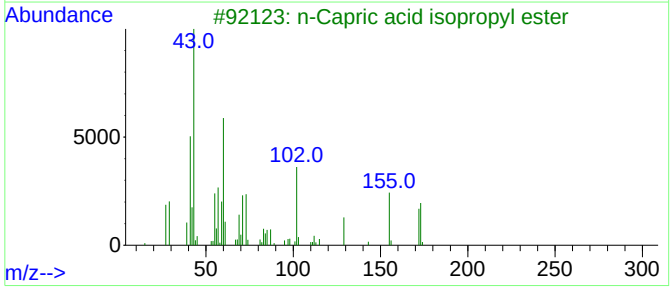


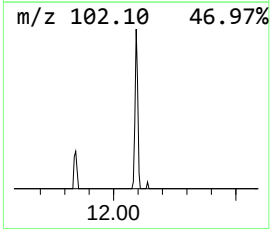












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Data File : BF136737.D
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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

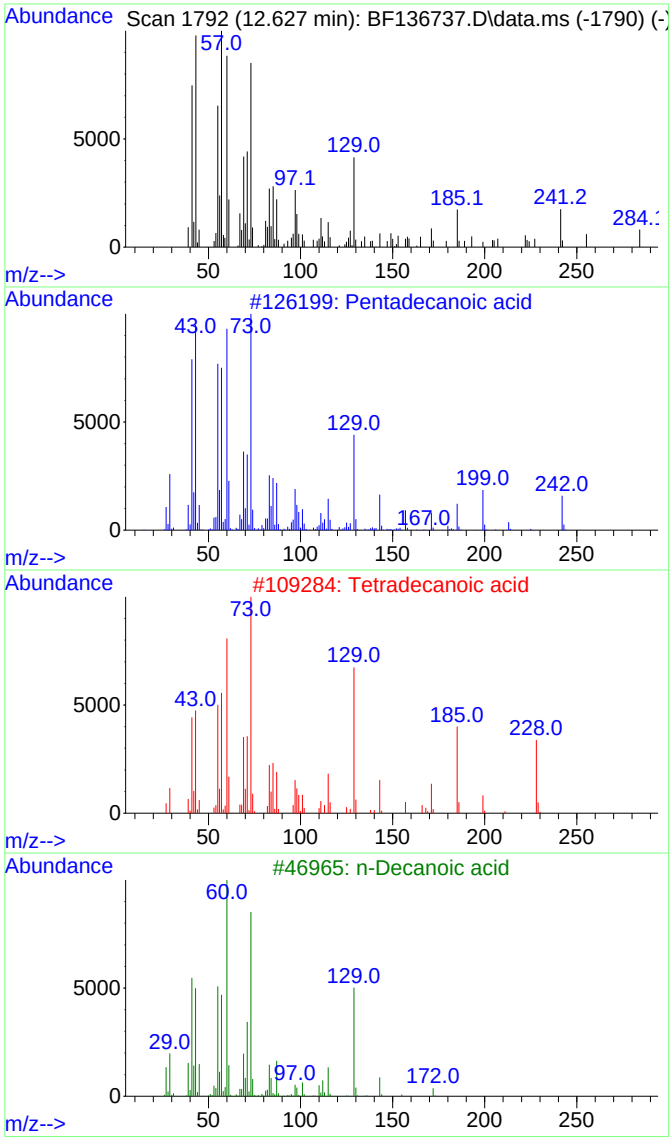
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

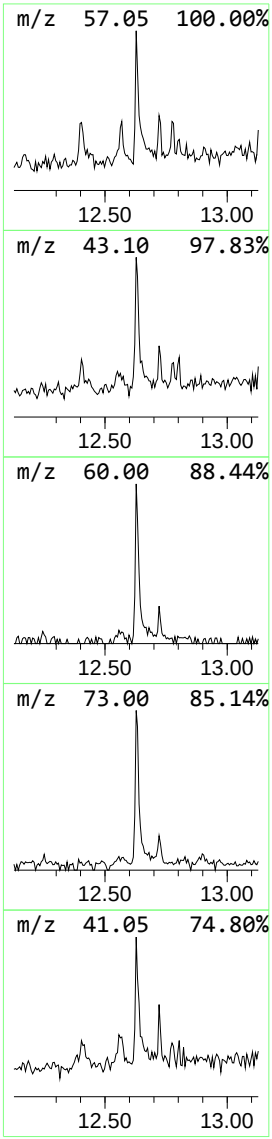
****

Peak Number 6 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.627	4.04 ng	89852	Phenanthrene-d10	11.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	n-Decanoic acid	172	C10H20O2	000334-48-5	64
4	Octadecanoic acid	284	C18H36O2	000057-11-4	46
5	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	20





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Data File : BF136737.D
Acq On : 27 Dec 2023 00:40
Operator : CG\JU
Sample : 05812-01RE
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW2RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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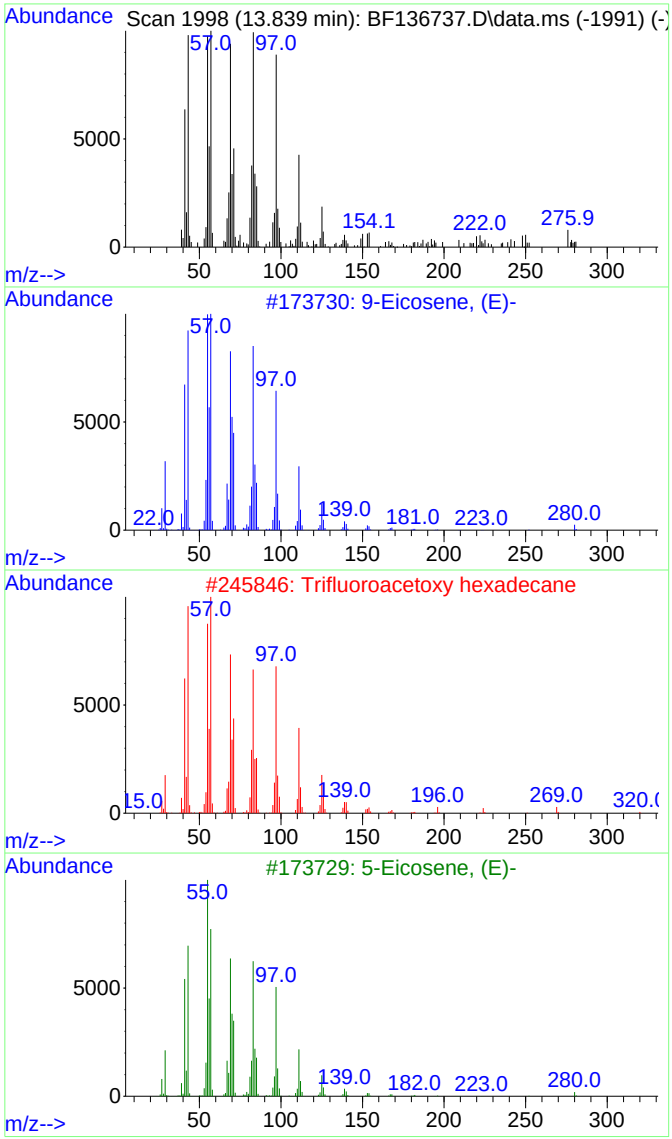
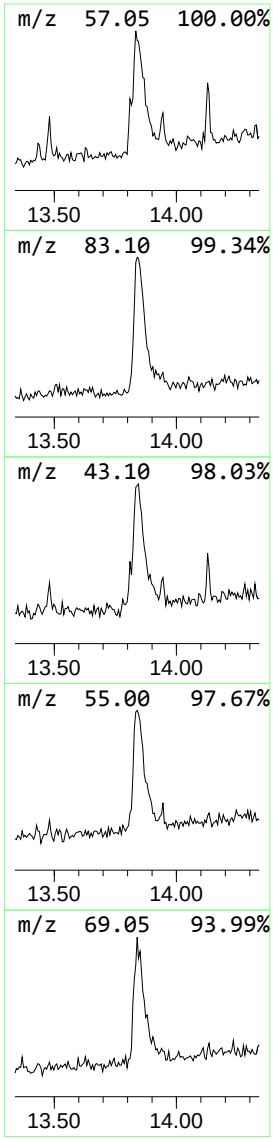
Peak Number 7 9-Eicosene, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	16.54 ng	360381	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	90
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	87
5	1-Heneicosanol	312	C21H44O	015594-90-8	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136737.D
Acq On : 27 Dec 2023 00:40
Operator : CG\JU
Sample : 05812-01RE
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW2RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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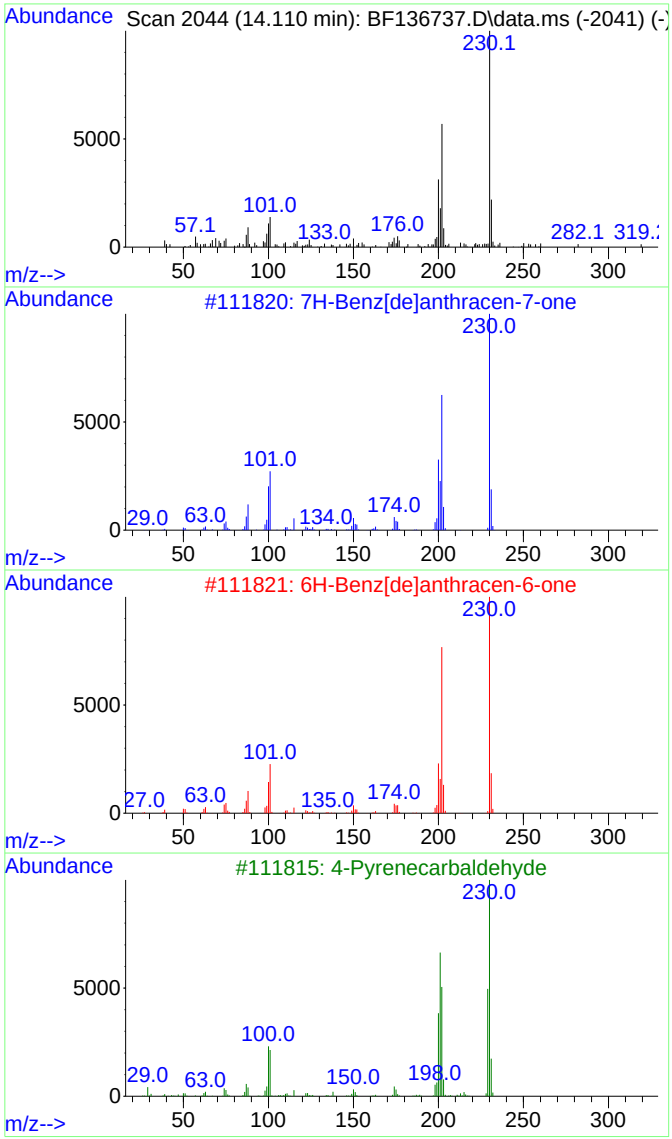
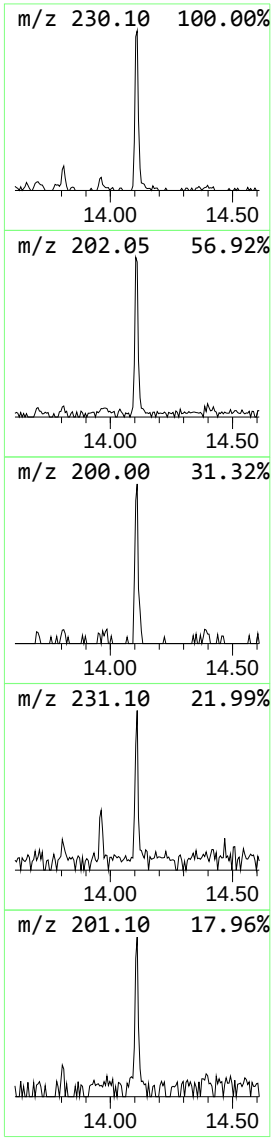
Peak Number 8 7H-Benz[de]anthracen-7-one Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.110	2.11 ng	45902	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	95
2	6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	87
3	4-Pyrenecarbaldehyde	230	C17H10O	022245-51-8	70
4	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	68
5	1-Pyrenecarboxaldehyde	230	C17H10O	003029-19-4	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136737.D
Acq On : 27 Dec 2023 00:40
Operator : CG\JU
Sample : 05812-01RE
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW2RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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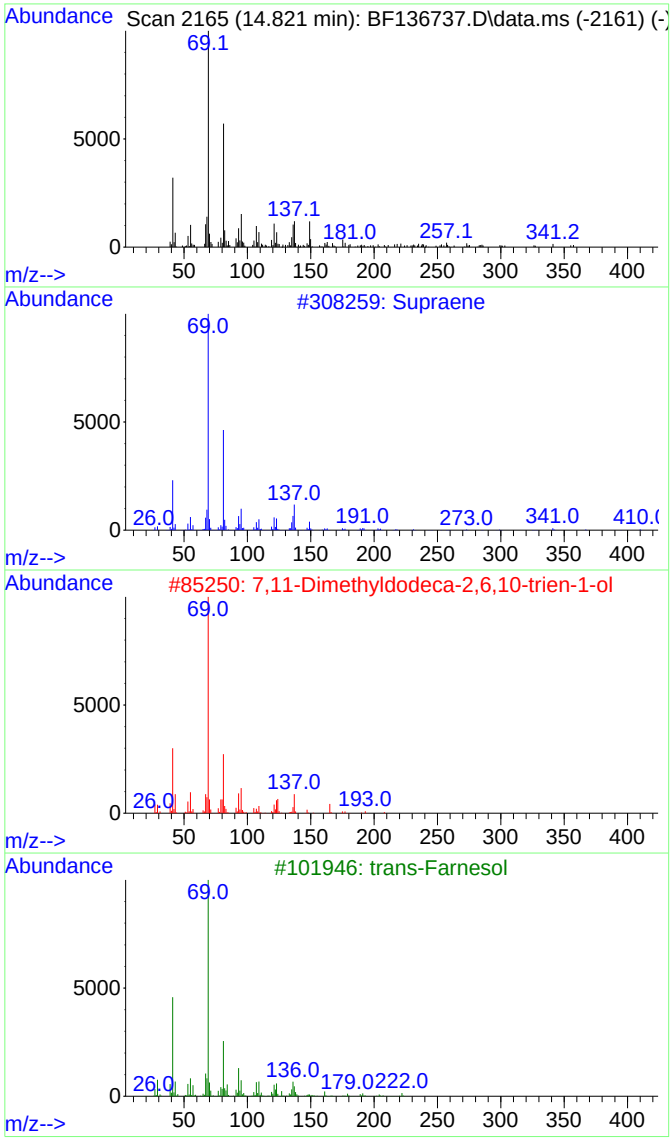
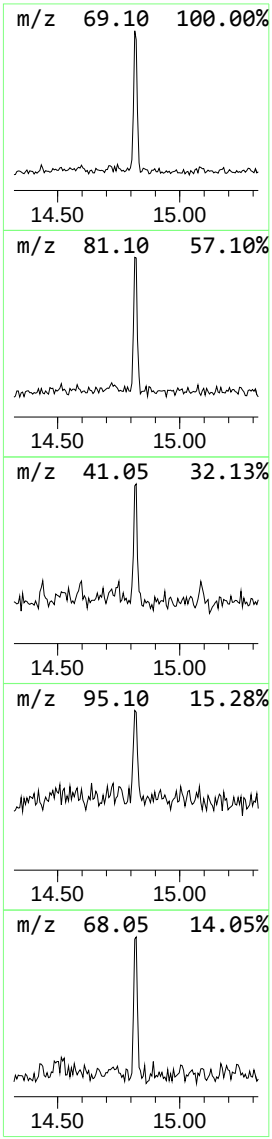
Peak Number 9 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.821	6.43 ng	112060	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	83
2	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	68
3	trans-Farnesol	222	C15H26O	000106-28-5	59
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	59
5	(3E,7E)-4,8,12-Trimethyltrideca-...	218	C16H26	062235-06-7	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136737.D
Acq On : 27 Dec 2023 00:40
Operator : CG\JU
Sample : 05812-01RE
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW2RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
1-Phenoxypropan...	8.375	3.4	ng	89514	2	8.057	526590	20.0
unknown9.916	9.916	5.5	ng	143828	3	9.816	522210	20.0
n-Hexadecanoic ...	11.845	16.5	ng	367605	4	11.304	444941	20.0
Isopropyl palmi...	12.092	2.7	ng	60447	4	11.304	444941	20.0
Pentadecanoic acid	12.627	4.0	ng	89852	4	11.304	444941	20.0
9-Eicosene, (E)-	13.839	16.5	ng	360381	5	13.963	435845	20.0
7H-Benz[de]anth...	14.110	2.1	ng	45902	5	13.963	435845	20.0
Supraene	14.821	6.4	ng	112060	6	15.439	348444	20.0