LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092123\
Data File : BF135384.D
Acq On : 21 Sep 2023 17:09
Operator : CG\JU
Sample : 04515-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

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-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135384.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.981	489	492	503	rVB	52852	71569	2.82%	0.351%
2	5.387	557	561	582	rBV	2495527	2464921	97.17%	12.081%
3	6.028	667	670	674	rBV	172402	154740	6.10%	0.758%
4	6.405	729	734	740	rBV	2370405	2536739	100.00%	12.433%
5	6.452	740	742	746	rVB	238271	195663	7.71%	0.959%
6	6.757	790	794	805	rVB	1053431	872041	34.38%	4.274%
7	7.322	885	890	893	rBV	1785571	1595337	62.89%	7.819%
8	7.352	893	895	901	rVB	255939	202034	7.96%	0.990%
9	8.034	1007	1011	1015	rBV	1274781	1049958	41.39%	5.146%
10	9.110	1190	1194	1206	rBV	2638212	2500548	98.57%	12.256%
11	9.234	1210	1215	1219	rBV	53309	59203	2.33%	0.290%
12	9.710	1293	1296	1303	rVB	224594	188619	7.44%	0.924%
13	9.793	1306	1310	1320	rVB	1135799	994966	39.22%	4.877%
14	10.587	1441	1445	1457	rBV	1109153	1156138	45.58%	5.667%
15	11.240	1553	1556	1560	rBV2	30690	36927	1.46%	0.181%
16	11.281	1560	1563	1566	rVV	917270	842658	33.22%	4.130%
17	11.304	1566	1567	1571	rVB	87019	64836	2.56%	0.318%
18	11.751	1639	1643	1646	rBV4	26480	32551	1.28%	0.160%
19	11.787	1646	1649	1652	rVV2	68478	72511	2.86%	0.355%
20	11.822	1652	1655	1665	rVB3	462433	483923	19.08%	2.372%
21	11.998	1682	1685	1694	rBV6	24989	37892	1.49%	0.186%
22	12.392	1746	1752	1755	rBV4	28139	47058	1.86%	0.231%
23	12.504	1765	1771	1774	rBV	154729	154808	6.10%	0.759%
24	12.551	1774	1779	1784	rVV6	40414	94339	3.72%	0.462%
25	12.610	1786	1789	1800	rVV2	102935	162749	6.42%	0.798%
26	12.734	1804	1810	1813	rVV	138889	127471	5.02%	0.625%
27	12.881	1831	1835	1838	rBV	1971561	1720346	67.82%	8.432%
28	13.045	1859	1863	1865	rBV4	17321	25894	1.02%	0.127%
29	13.075	1865	1868	1871	rVB2	42287	54236	2.14%	0.266%
30	13.175	1881	1885	1888	rBV2	22609	29877	1.18%	0.146%
31	13.369	1913	1918	1921	rBV	107219	123331	4.86%	0.604%
32	13.398	1921	1923	1928	rVB	108913	109741	4.33%	0.538%
33	13.581	1951	1954	1958	rVB2	37131	37147	1.46%	0.182%
34	13.645	1962	1965	1968	rBV3	78819	86659	3.42%	0.425%
35	13.792	1987	1990	1993	rVB	50600	49812	1.96%	0.244%
36	13.886	2001	2006	2008	rBV2	81714	136875	5.40%	0.671%

LSC Area Percent Report

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Acq On : 21 Sep 2023 17:09
Operator : CG\JU
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

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-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.939	2011	2015	2018	rVB	827498	763191	30.09%	3.741%
38	14.110	2041	2044	2051	rVB4	28986	34889	1.38%	0.171%
39	14.416	2093	2096	2100	rVB	53168	49670	1.96%	0.243%
40	14.792	2158	2160	2163	rVB	33562	29846	1.18%	0.146%
41	14.863	2170	2172	2177	rVB4	31742	36092	1.42%	0.177%
42	14.980	2189	2192	2195	rBV	39206	53884	2.12%	0.264%
43	15.057	2202	2205	2208	rVB	90757	98022	3.86%	0.480%
44	15.345	2251	2254	2258	rVB2	42967	53007	2.09%	0.260%
45	15.404	2260	2264	2279	rVB	452001	620557	24.46%	3.042%
46	15.875	2340	2344	2349	rVB	61049	89403	3.52%	0.438%

Sum of corrected areas: 20402678

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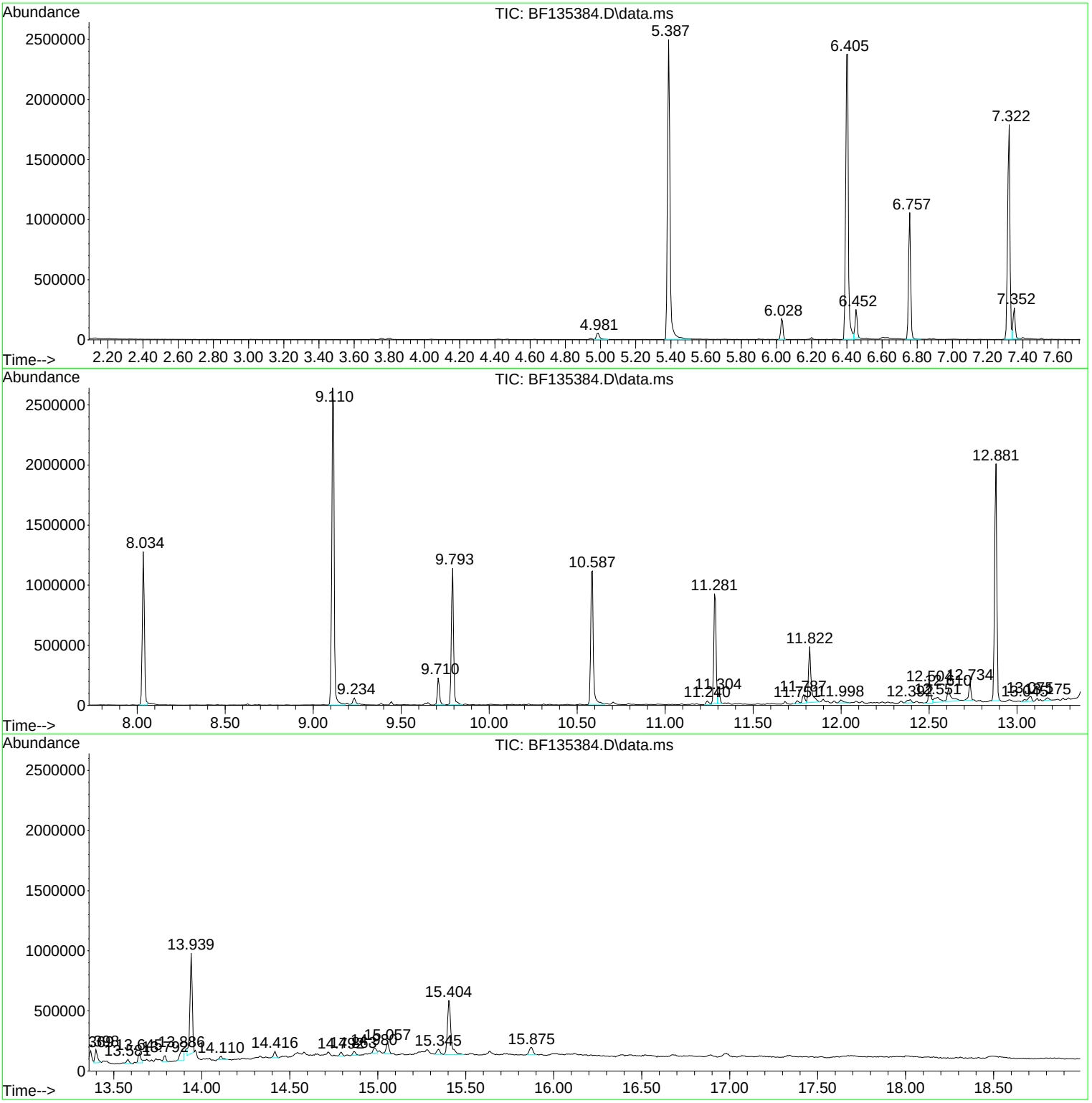
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF135384.D
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Operator : CG\JU
Sample : 04515-01
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BNA_F
ClientSampleId :
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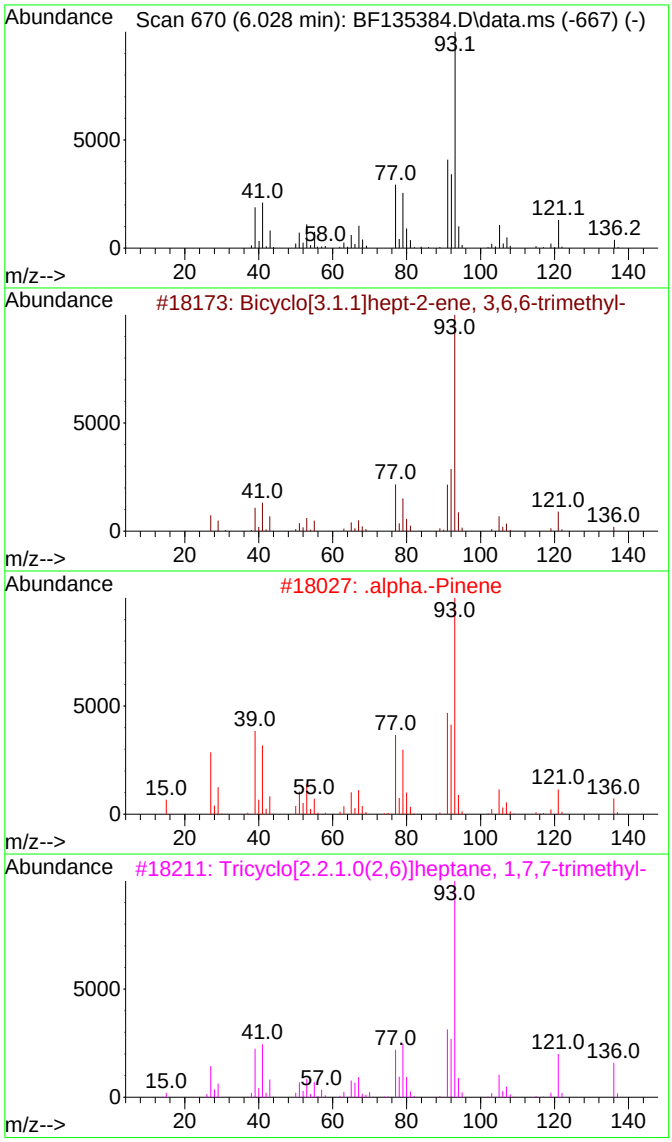
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

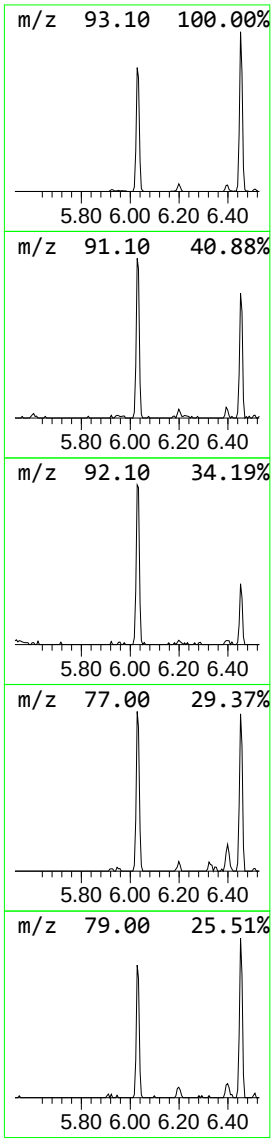
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Bicyclo[3.1.1]hept-2-ene, 3... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.028	3.55 ng	154740	1,4-Dichlorobenzene-d4	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	94
2	.alpha.-Pinene	136	C10H16	000080-56-8	94
3	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91
4	.gamma.-Terpinene	136	C10H16	000099-85-4	87
5	1,3,6-Octatriene, 3,7-dimethyl-,...	136	C10H16	003338-55-4	87





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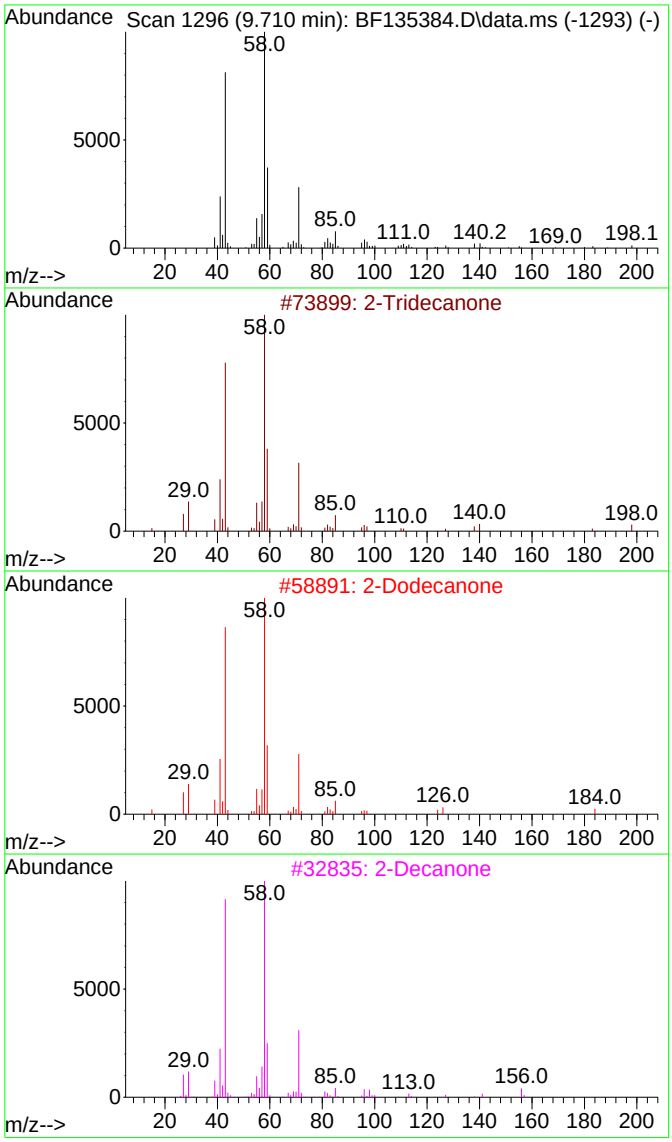
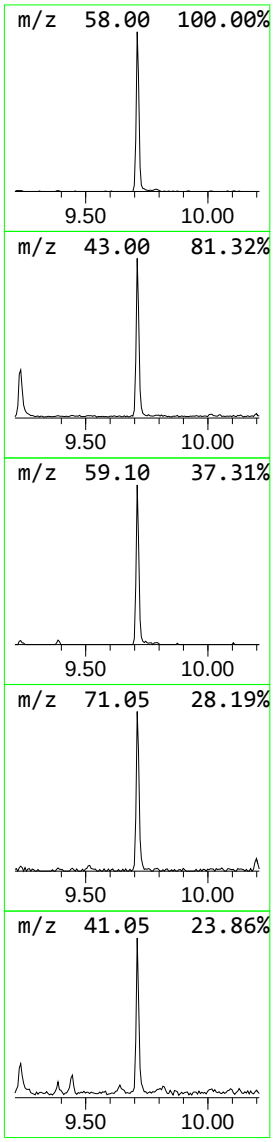
****

Peak Number 2 2-Tridecanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.710	3.79 ng	188619	Acenaphthene-d10	9.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Tridecanone	198	C13H26O	000593-08-8	97
2	2-Dodecanone	184	C12H24O	006175-49-1	90
3	2-Decanone	156	C10H20O	000693-54-9	83
4	2-Undecanone	170	C11H22O	000112-12-9	83
5	2-Nonanone	142	C9H18O	000821-55-6	72





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

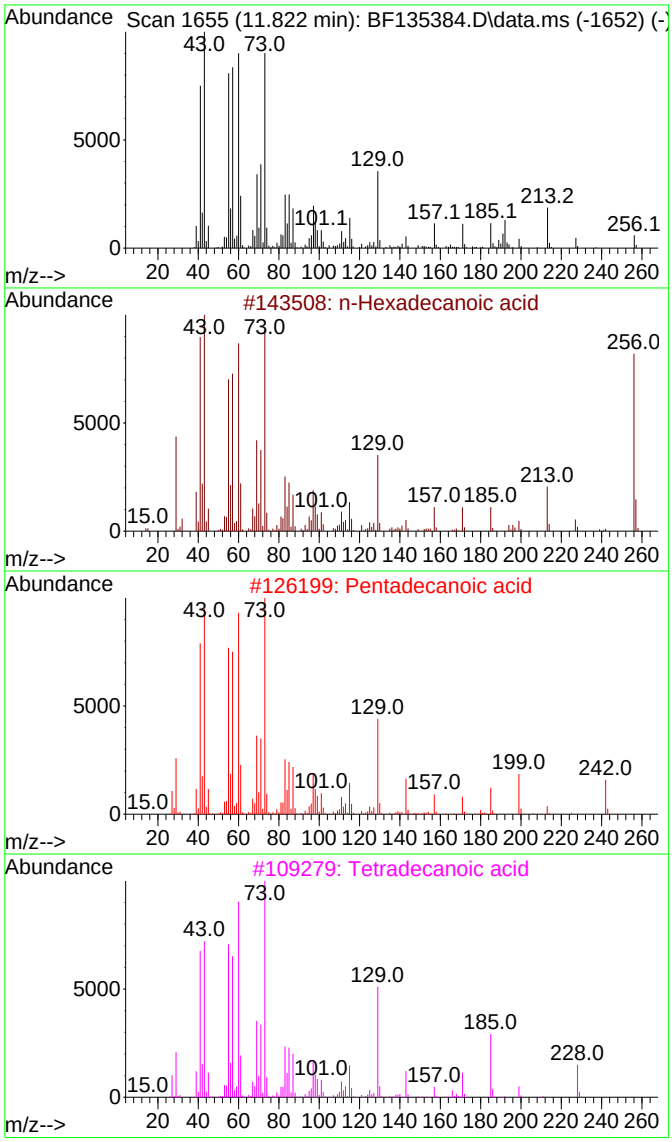
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

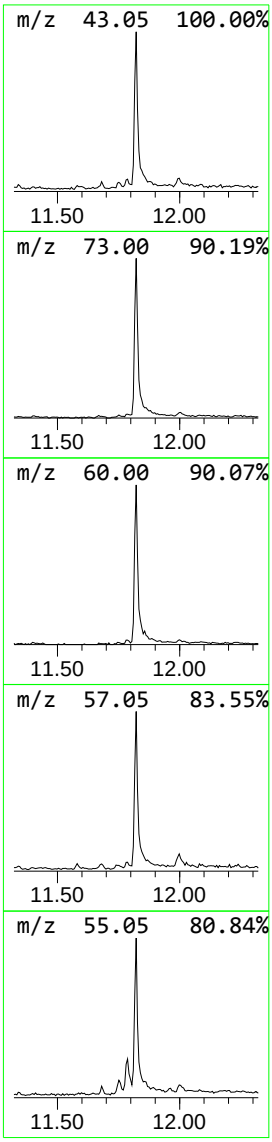
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.822	11.49 ng	483923	Phenanthrene-d10	11.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	78
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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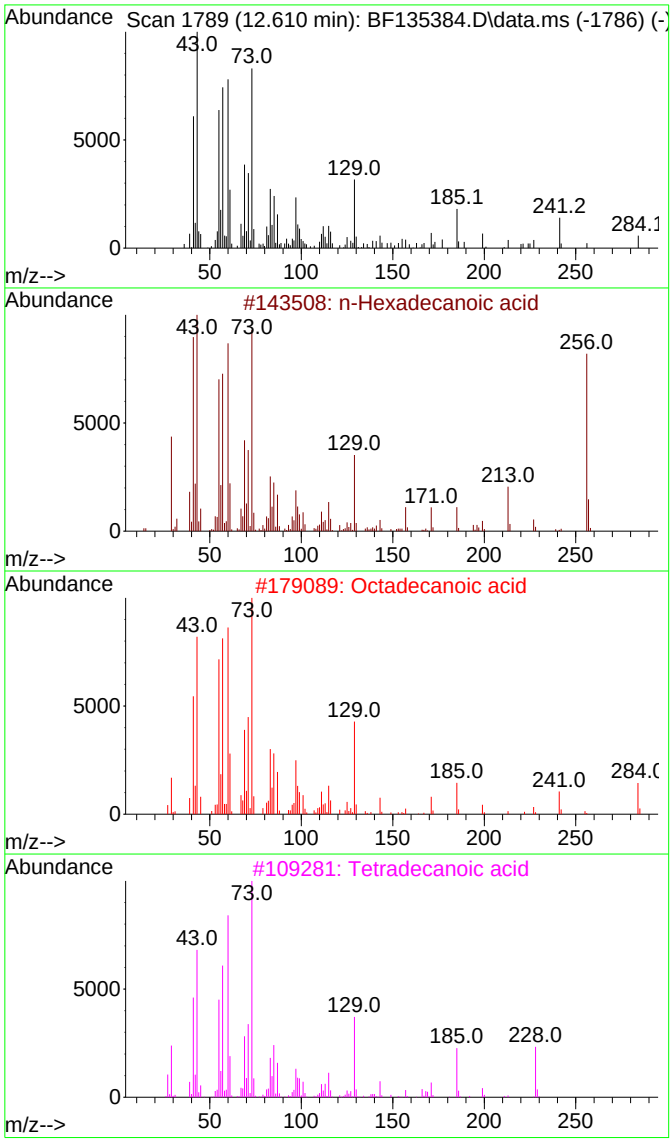
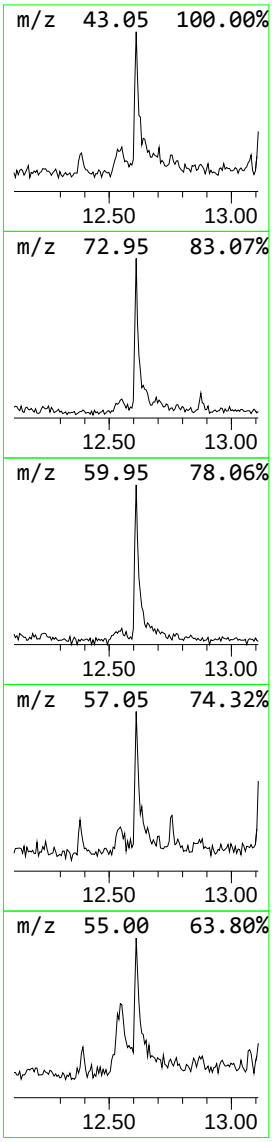
Peak Number 4 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	4.26 ng	162749	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Octadecanoic acid	284	C18H36O2	000057-11-4	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





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Sample : 04515-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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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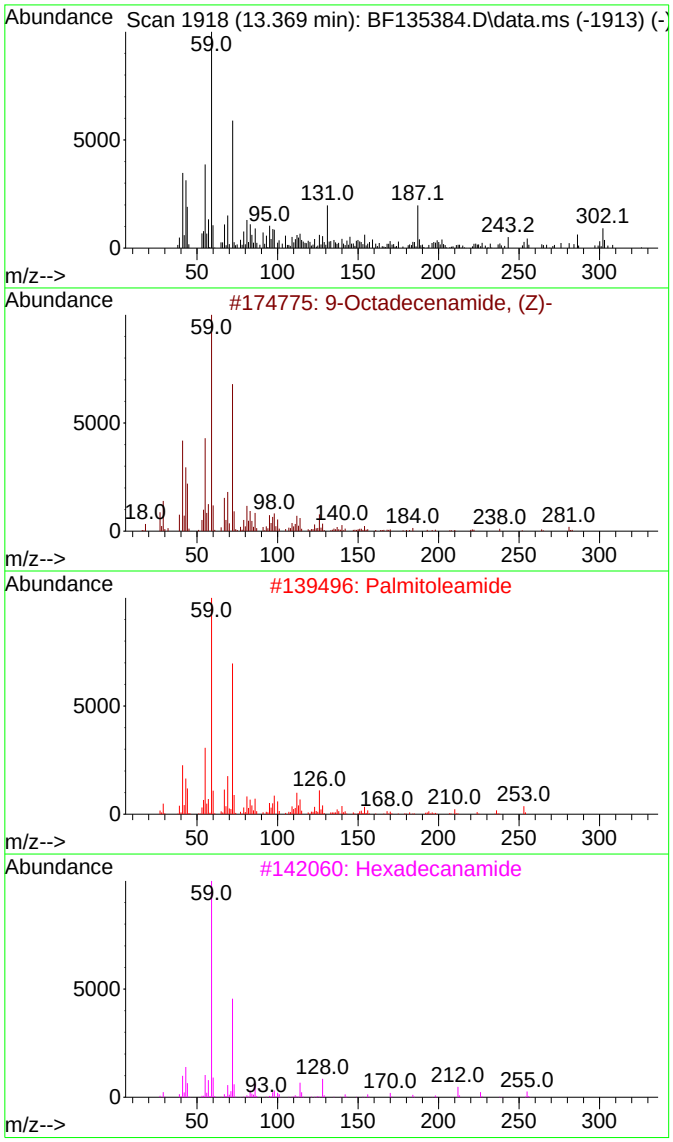
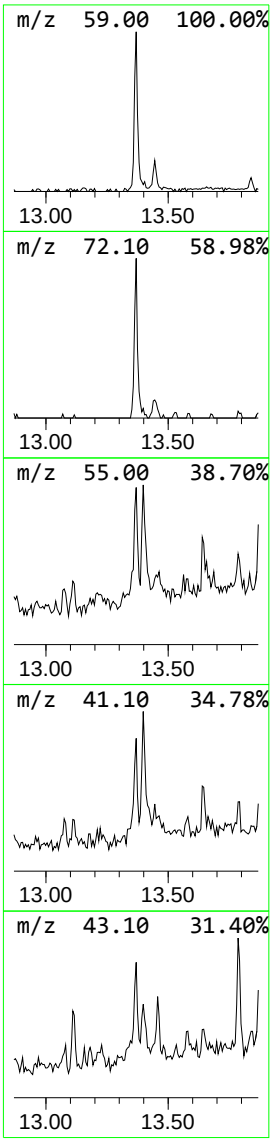
Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.369	3.23 ng	123331	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	92
2	Palmitoleamide	253	C16H31NO	106010-22-4	78
3	Hexadecanamide	255	C16H33NO	000629-54-9	60
4	Tetradecanamide	227	C14H29NO	000638-58-4	49
5	Enanthamide	129	C7H15NO	000628-62-6	35





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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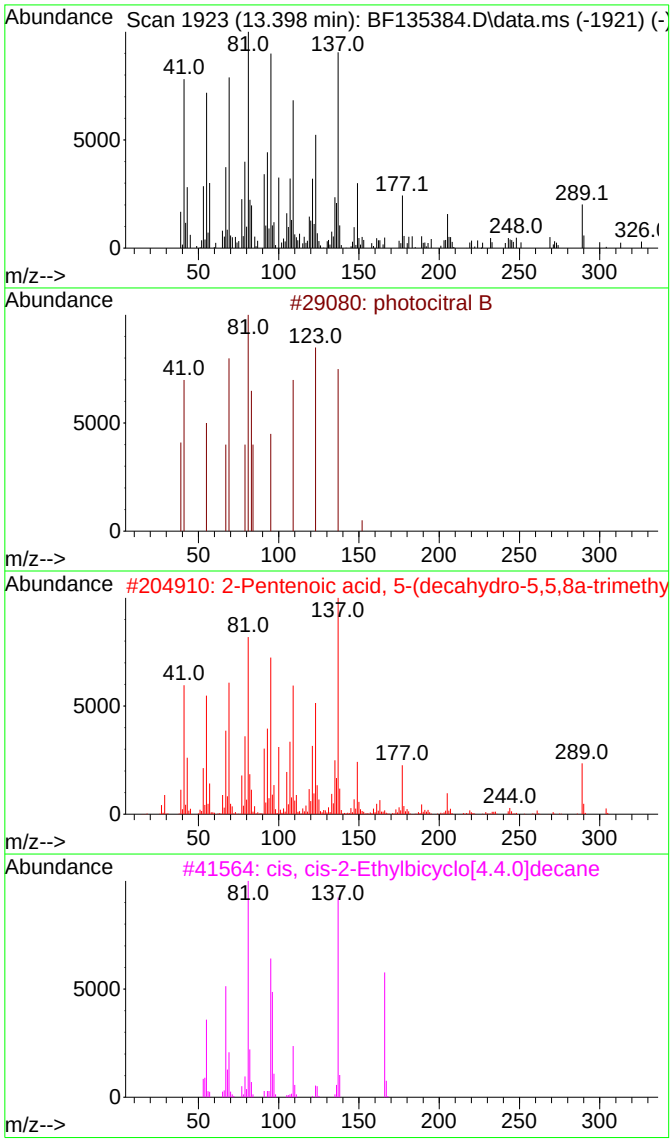
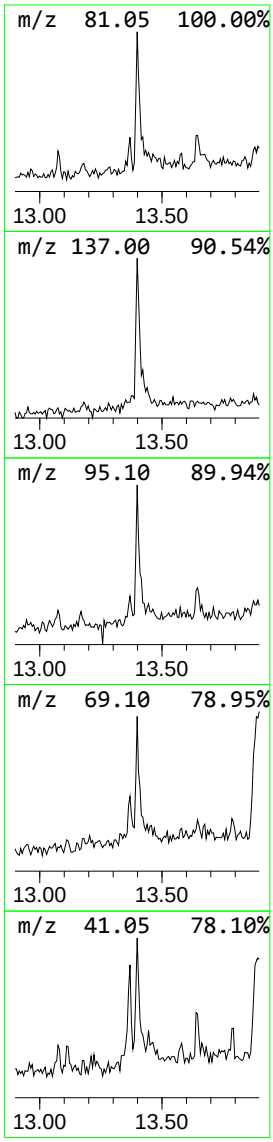
Peak Number 6 photocitral B Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.398	2.88 ng	109741	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	photocitral B	152	C10H16O	006040-45-5	64
2	2-Pentenoic acid, 5-(decahydro-5...	304	C20H32O2	024470-48-2	55
3	cis, cis-2-Ethylbicyclo[4.4.0]de...	166	C12H22	066660-40-0	49
4	cis, cis-3-Ethylbicyclo[4.4.0]de...	166	C12H22	066660-42-2	49
5	(E)-3-Methyl-5-((1R,4aR,8aR)-5,5...	304	C20H32O2	020257-75-4	46





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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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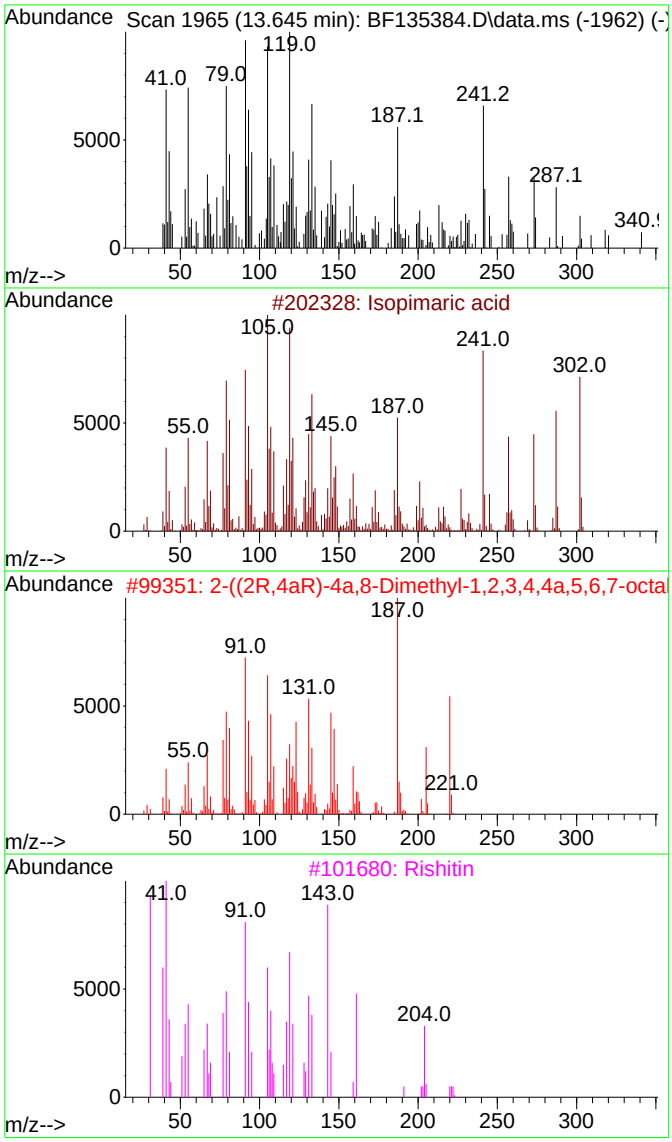
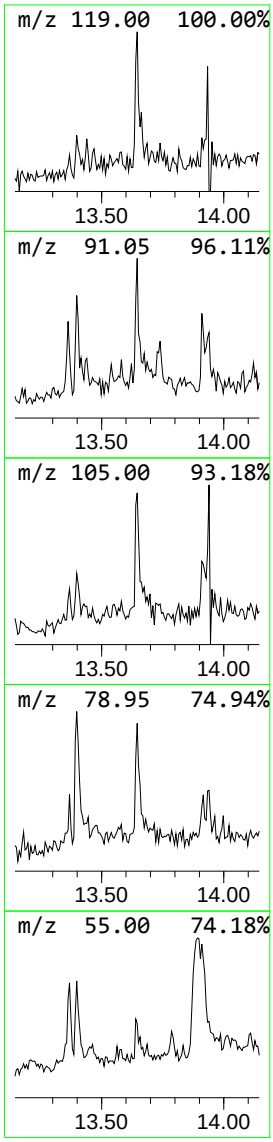
Peak Number 7 Isopimaric acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.645	2.27 ng	86659	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopimaric acid	302	C20H30O2	005835-26-7	95
2	2-((2R,4aR)-4a,8-Dimethyl-1,2,3,...	220	C15H24O	065018-14-6	38
3	Rishitin	222	C14H22O2	018178-54-6	35
4	Androst-5-en-3-ol, 4,4-dimethyl-...	302	C21H34O	007673-17-8	25
5	Andrographolide	350	C20H30O5	005508-58-7	18





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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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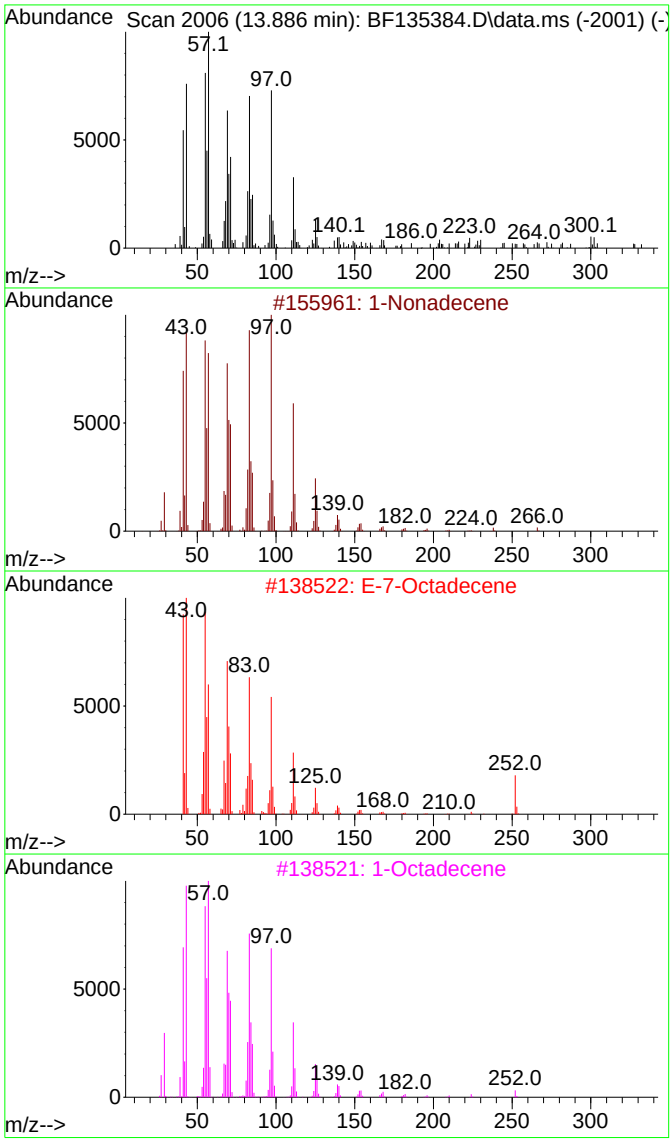
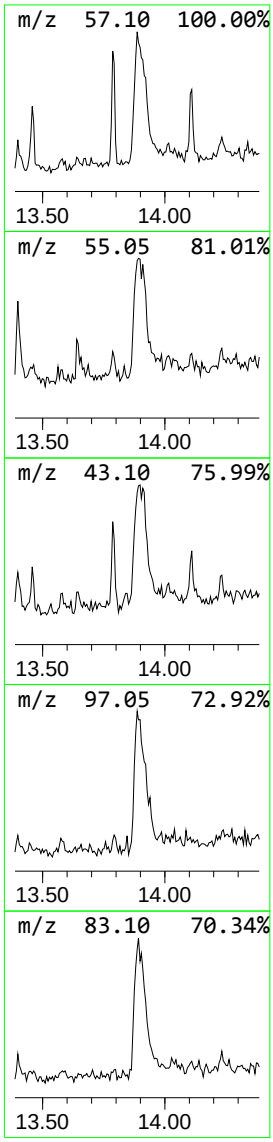
Peak Number 8 1-Nonadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	3.59 ng	136875	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	94
2	E-7-Octadecene	252	C18H36	1000130-92-0	93
3	1-Octadecene	252	C18H36	000112-88-9	93
4	1-Docosene	308	C22H44	001599-67-3	93
5	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	90





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BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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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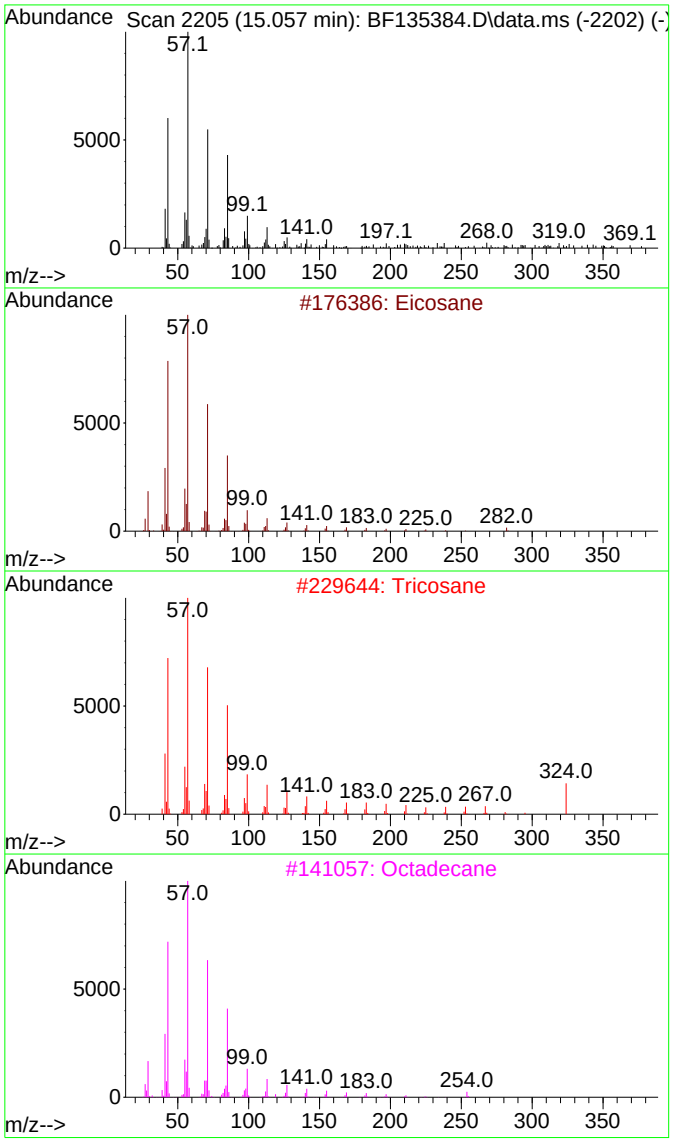
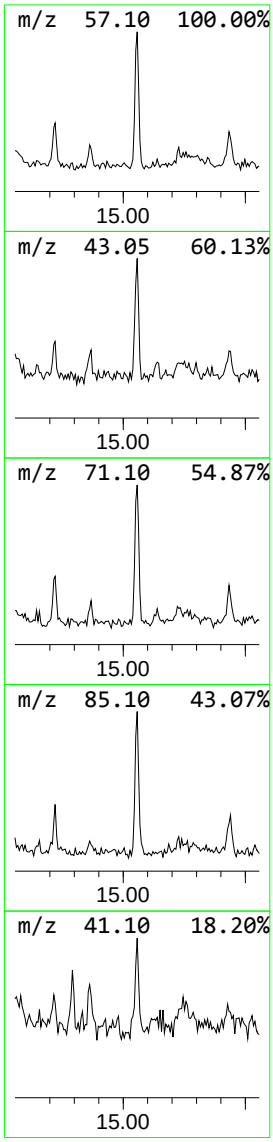
Peak Number 9 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.057	3.16 ng	98022	Perylene-d12	15.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Tricosane	324	C23H48	000638-67-5	90
3	Octadecane	254	C18H38	000593-45-3	87
4	Nonadecane	268	C19H40	000629-92-5	87
5	Hexacosane	366	C26H54	000630-01-3	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092123\
Data File : BF135384.D
Acq On : 21 Sep 2023 17:09
Operator : CG\JU
Sample : 04515-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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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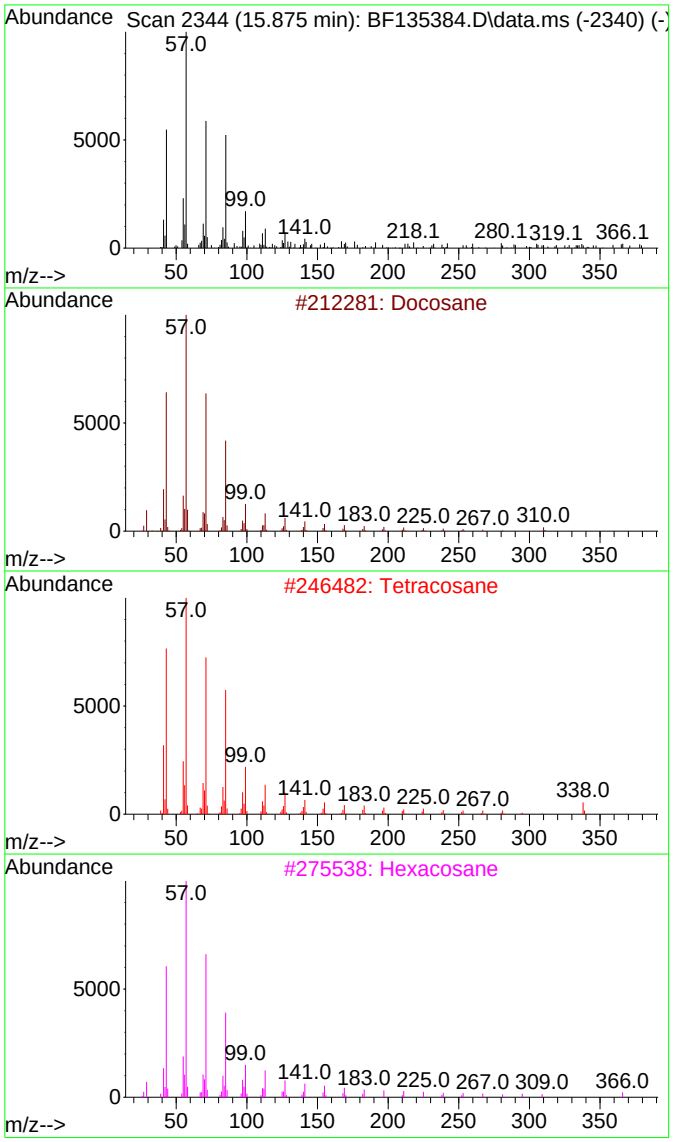
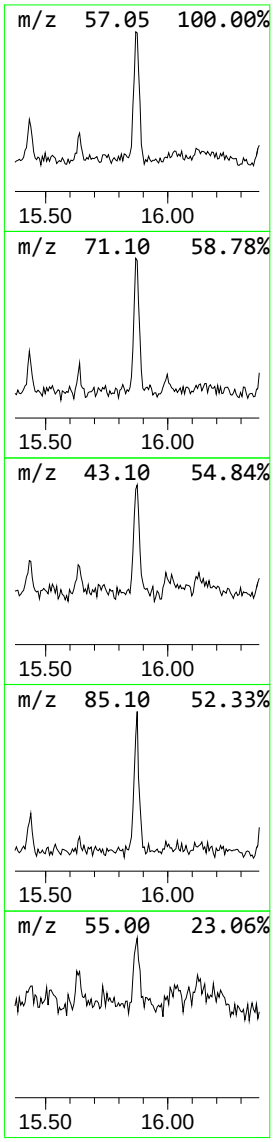
Peak Number 10 Docosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.874	2.88 ng	89403	Perylene-d12	15.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	93
2	Tetracosane	338	C24H50	000646-31-1	93
3	Hexacosane	366	C26H54	000630-01-3	89
4	Tricosane, 2-methyl-	338	C24H50	001928-30-9	87
5	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092123\
Data File : BF135384.D
Acq On : 21 Sep 2023 17:09
Operator : CG\JU
Sample : 04515-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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
Bicyclo[3.1.1]h...	6.028	3.5	ng	154740	1	6.757	872041	20.0
2-Tridecanone	9.710	3.8	ng	188619	3	9.793	994966	20.0
n-Hexadecanoic ...	11.822	11.5	ng	483923	4	11.281	842658	20.0
Octadecanoic acid	12.610	4.3	ng	162749	5	13.939	763191	20.0
9-Octadecenamid...	13.369	3.2	ng	123331	5	13.939	763191	20.0
photocitral B	13.398	2.9	ng	109741	5	13.939	763191	20.0
Isopimaric acid	13.645	2.3	ng	86659	5	13.939	763191	20.0
1-Nonadecene	13.886	3.6	ng	136875	5	13.939	763191	20.0
Eicosane	15.057	3.2	ng	98022	6	15.404	620557	20.0
Docosane	15.874	2.9	ng	89403	6	15.404	620557	20.0