LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
Data File : BF123442.D
Acq On : 24 Mar 2021 16:46
Operator : JU/CG
Sample : M1777-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 248-250

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-BF032321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123442.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	17	24	29	rBV	1295900	1593666	19.41%	1.925%
2	5.534	580	586	589	rBV	4198131	4370479	53.24%	5.280%
3	5.869	635	643	649	rVB2	115581	187582	2.28%	0.227%
4	6.534	750	756	759	rBV	4345991	4484673	54.63%	5.418%
5	6.916	817	821	824	rBV	1539993	1284259	15.64%	1.552%
6	7.475	906	916	918	rBV	3030216	3012628	36.70%	3.640%
7	7.516	918	923	926	rVV	665052	647127	7.88%	0.782%
8	7.551	926	929	934	rVB5	176000	214108	2.61%	0.259%
9	7.951	993	997	1001	rVB5	88699	147694	1.80%	0.178%
10	8.151	1027	1031	1034	rBV4	89719	143949	1.75%	0.174%
11	8.198	1034	1039	1042	rVV	1968297	2006362	24.44%	2.424%
12	8.257	1046	1049	1052	rVB3	254541	290469	3.54%	0.351%
13	8.286	1052	1054	1057	rBV3	137355	146001	1.78%	0.176%
14	8.439	1076	1080	1082	rBV3	146708	151481	1.85%	0.183%
15	8.492	1086	1089	1092	rVV4	259830	295948	3.60%	0.358%
16	8.551	1096	1099	1101	rVB3	157354	142240	1.73%	0.172%
17	8.586	1101	1105	1108	rBV4	173024	233982	2.85%	0.283%
18	8.622	1108	1111	1113	rBV	343277	320647	3.91%	0.387%
19	8.663	1117	1118	1122	rVB2	305764	258803	3.15%	0.313%
20	8.704	1122	1125	1128	rBV2	299674	296407	3.61%	0.358%
21	8.751	1128	1133	1137	rBV6	200235	412871	5.03%	0.499%
22	8.792	1137	1140	1142	rBV2	341776	315791	3.85%	0.382%
23	8.892	1154	1157	1159	rBV3	268482	229660	2.80%	0.277%
24	8.951	1164	1167	1169	rBV3	299333	250201	3.05%	0.302%
25	8.980	1169	1172	1175	rBV3	229488	355877	4.33%	0.430%
26	9.027	1175	1180	1181	rBV2	232118	307094	3.74%	0.371%
27	9.045	1181	1183	1187	rVB4	211201	174791	2.13%	0.211%
28	9.080	1187	1189	1193	rBV5	294671	449387	5.47%	0.543%
29	9.116	1193	1195	1198	rVB4	230344	221777	2.70%	0.268%
30	9.198	1207	1209	1211	rBV	499513	425071	5.18%	0.514%
31	9.227	1211	1214	1218	rVB	942331	844388	10.29%	1.020%
32	9.280	1218	1223	1225	rBV	4633086	4532620	55.21%	5.476%
33	9.363	1233	1237	1242	rBV3	1439044	1873154	22.82%	2.263%
34	9.592	1274	1276	1279	rBV3	635765	724447	8.82%	0.875%
35	9.622	1279	1281	1282	rBV	393945	281459	3.43%	0.340%
36	9.639	1282	1284	1287	rVB3	707534	707346	8.62%	0.855%

LSC Area Percent Report

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Operator : JU/CG
Sample : M1777-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 248-250

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-BF032321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	9.674	1287	1290	1291	rBV2	2484501	2084972	25.40%	2.519%
38	9.780	1304	1308	1314	rBV5	1026275	1343410	16.36%	1.623%
39	9.833	1314	1317	1320	rBV4	1445679	1813145	22.09%	2.190%
40	9.880	1322	1325	1327	rVB	2733865	2320926	28.27%	2.804%
41	9.963	1333	1339	1342	rBV5	2395281	3854953	46.96%	4.657%
42	10.163	1371	1373	1376	rVB2	837276	658342	8.02%	0.795%
43	10.227	1382	1384	1387	rBV2	1434758	1405258	17.12%	1.698%
44	10.286	1392	1394	1396	rBV2	887161	885329	10.78%	1.070%
45	10.345	1401	1404	1406	rBV3	855592	908613	11.07%	1.098%
46	10.386	1408	1411	1413	rBV	1706062	1610182	19.61%	1.945%
47	10.633	1450	1453	1457	rVB	2796805	2766046	33.69%	3.342%
48	10.757	1470	1474	1477	rBV3	2096982	2551738	31.08%	3.083%
49	10.904	1494	1499	1506	rBV	5632334	8209461	100.00%	9.918%
50	11.380	1577	1580	1586	rVB	4584402	5047139	61.48%	6.098%
51	13.057	1862	1865	1875	rVB	3432685	4433285	54.00%	5.356%
52	13.592	1954	1956	1959	rVB	870983	672761	8.19%	0.813%
53	13.945	2014	2016	2024	rVB	994491	1414862	17.23%	1.709%
54	14.110	2041	2044	2047	rVB	1048063	898491	10.94%	1.085%
55	14.598	2125	2127	2131	rVB2	492130	433759	5.28%	0.524%
56	15.562	2287	2291	2295	rBV	900350	1159729	14.13%	1.401%
57	15.609	2295	2299	2303	rVB	880976	1101410	13.42%	1.331%
58	16.162	2391	2393	2406	rVB4	204683	364117	4.44%	0.440%
59	16.362	2423	2427	2435	rVB	254818	499051	6.08%	0.603%
60	16.545	2451	2458	2467	rVB	1756892	3203374	39.02%	3.870%
61	16.821	2500	2505	2513	rVB	424097	798568	9.73%	0.965%

Sum of corrected areas: 82773360

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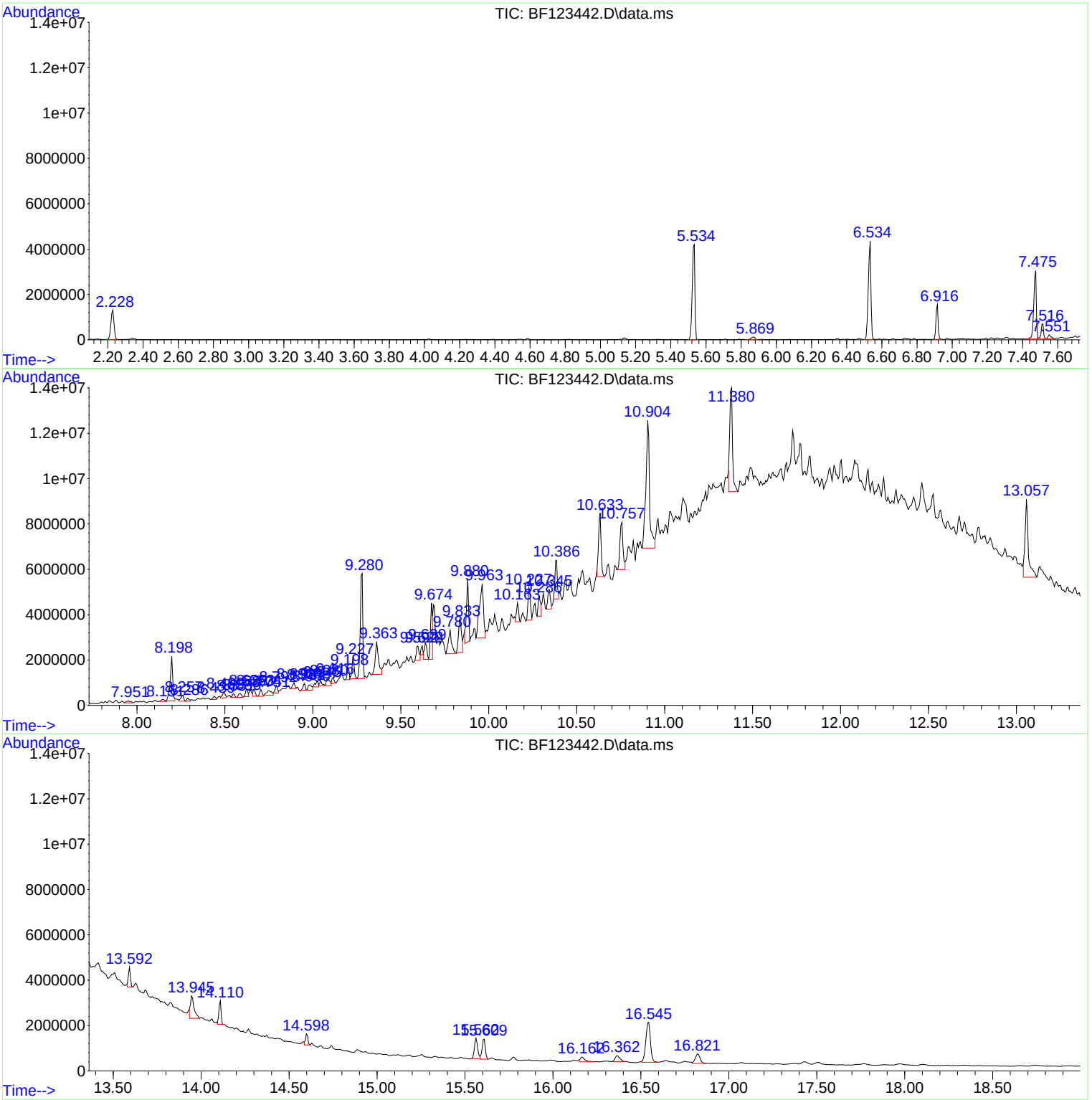
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
248-250

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF123442.D
Acq On : 24 Mar 2021 16:46
Operator : JU/CG
Sample : M1777-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 248-250

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
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TIC Library : C:\DATABASE\NIST11.L
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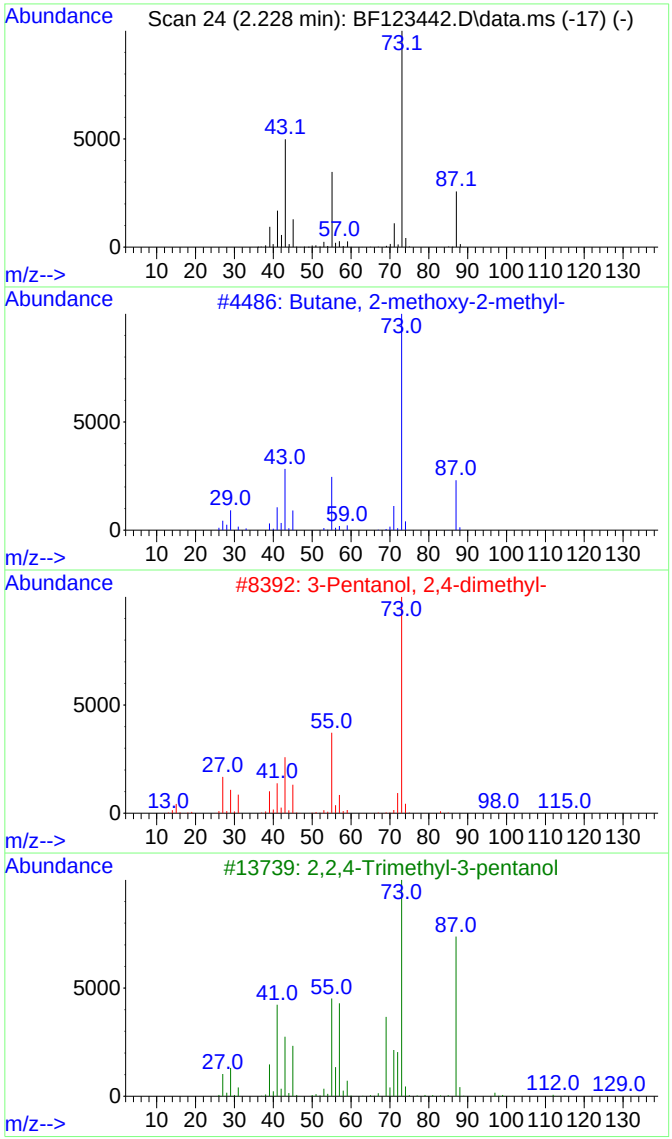
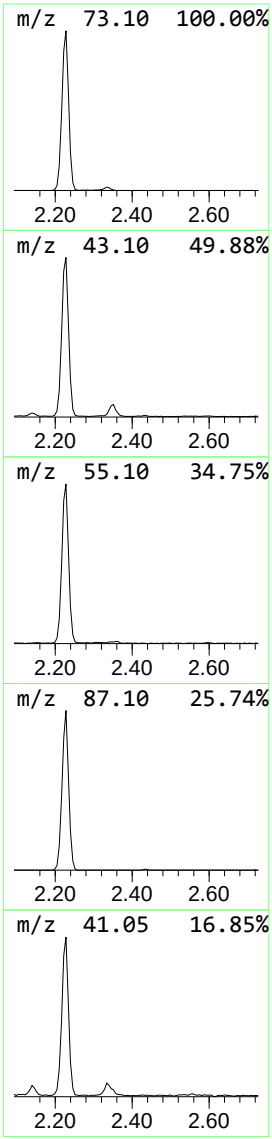
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	24.82 ng	1593670	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37





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Data File : BF123442.D
Acq On : 24 Mar 2021 16:46
Operator : JU/CG
Sample : M1777-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 248-250

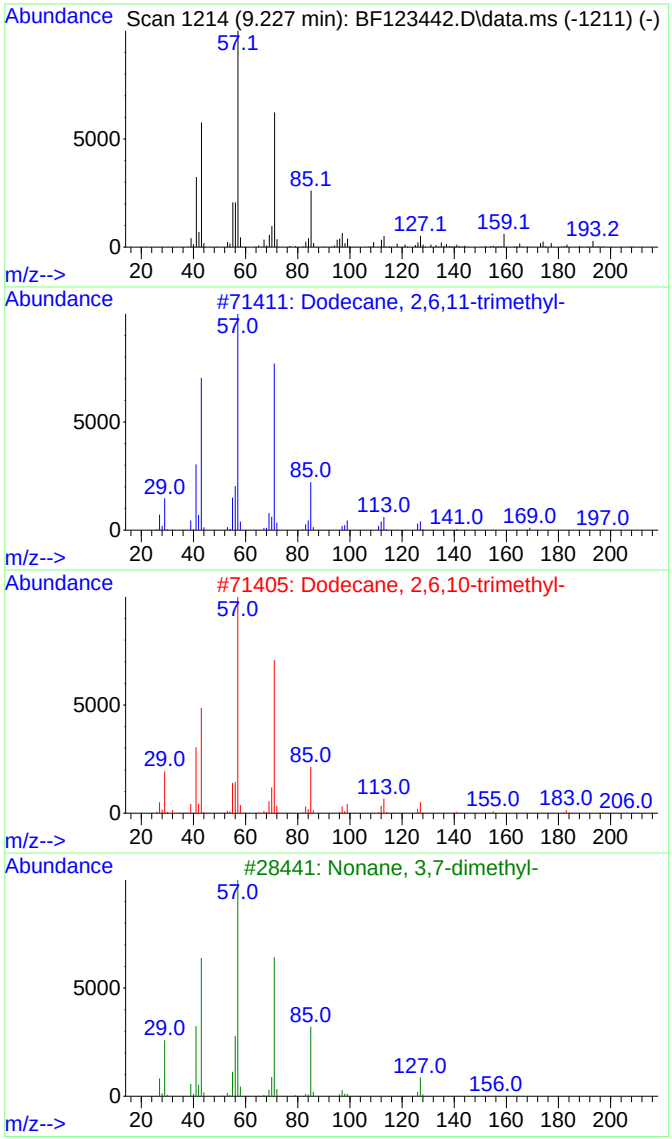
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

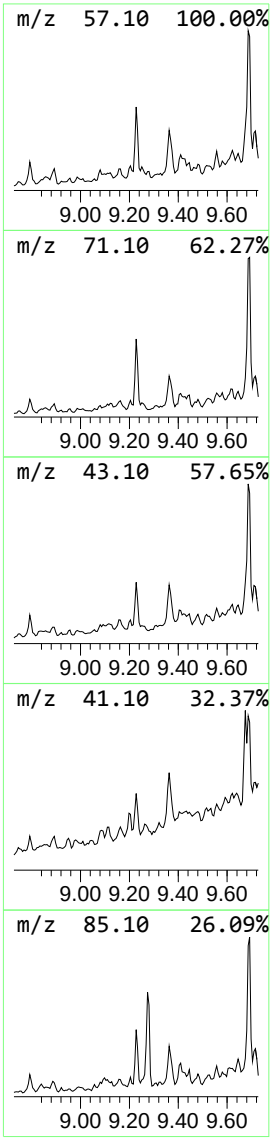
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Dodecane, 2,6,11-trimethyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.227	4.38 ng	844388	Acenaphthene-d10	9.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	72
2	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	64
3	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	64
4	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	58
5	Silane, trichlorodocosyl-	442	C22H45Cl3Si	007325-84-0	53





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Data File : BF123442.D
Acq On : 24 Mar 2021 16:46
Operator : JU/CG
Sample : M1777-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 248-250

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

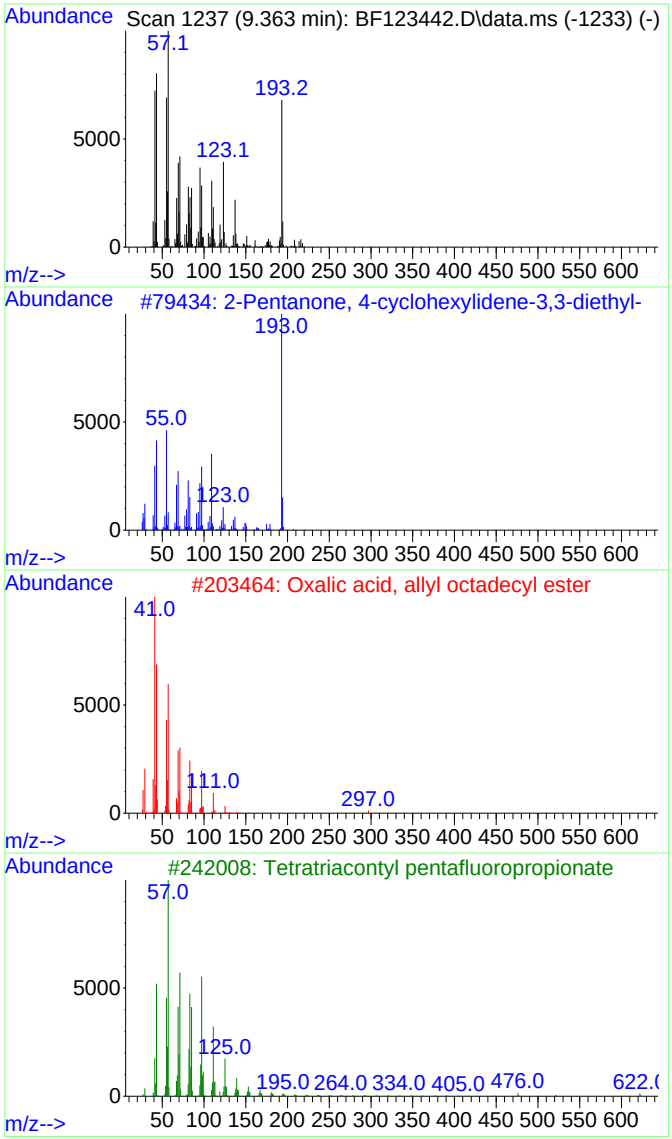
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

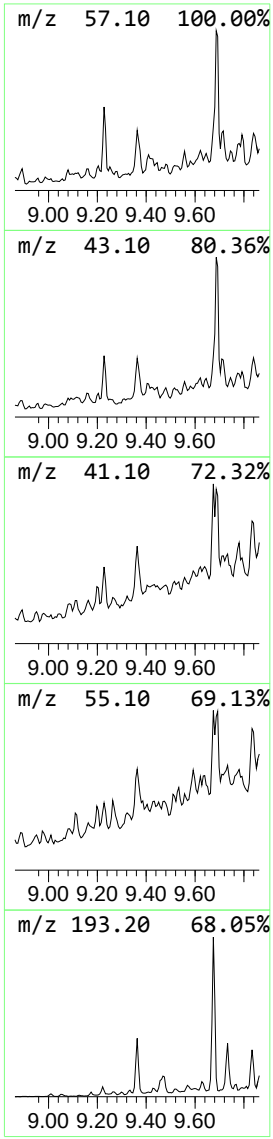
****

Peak Number 3 unknown9.363 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.363	9.72 ng	1873150	Acenaphthene-d10	9.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	38
2	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	25
3	Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	22
4	Oxalic acid, allyl undecyl ester	284	C16H28O4	1000309-23-9	22
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
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Acq On : 24 Mar 2021 16:46
Operator : JU/CG
Sample : M1777-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 248-250

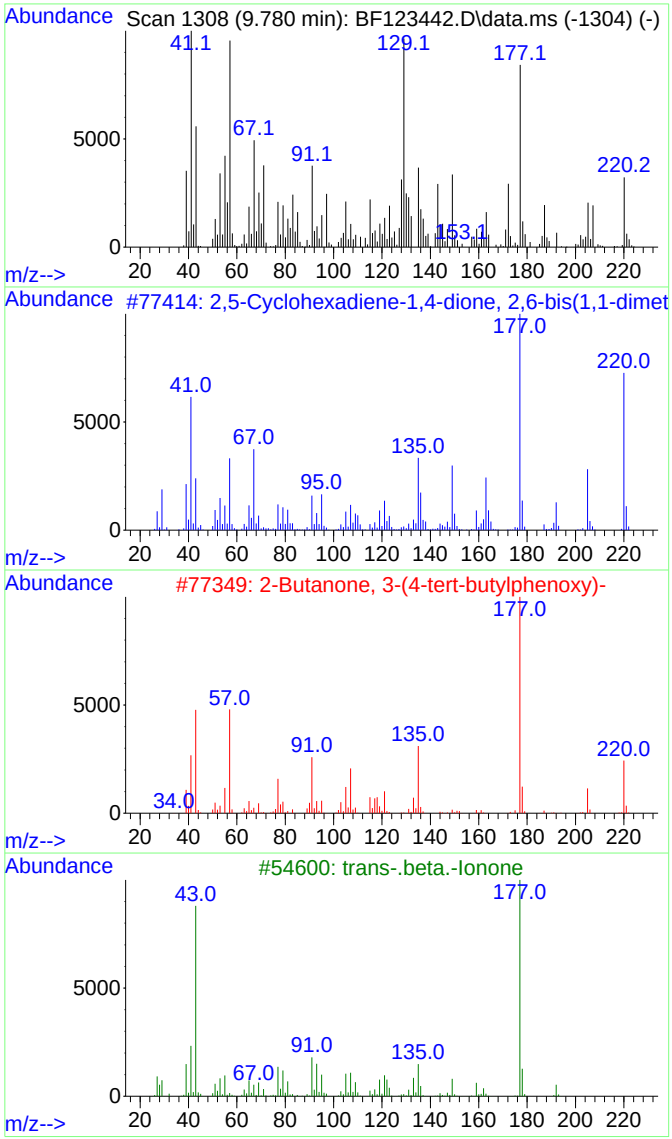
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

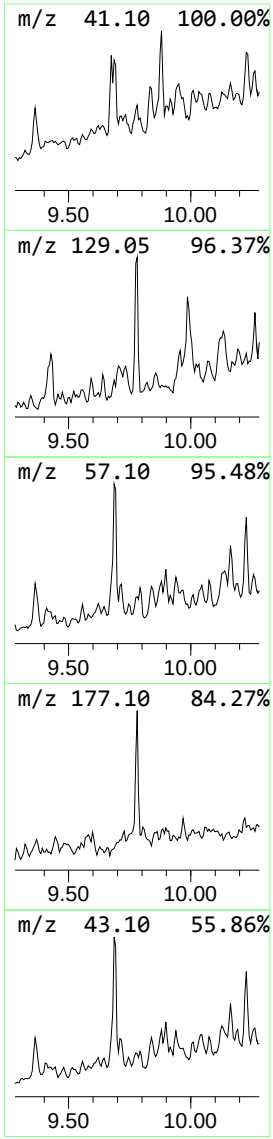
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.780	6.97 ng	1343410	Acenaphthene-d10	9.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	94
2	2-Butanone, 3-(4-tert-butylpheno...	220	C14H20O2	160875-28-5	38
3	trans-.beta.-Ionone	192	C13H20O	000079-77-6	35
4	(2-Thiobenzoyl)vinyl-methylamine	177	C10H11NS	024773-96-4	25
5	3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	20





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Operator : JU/CG
Sample : M1777-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 248-250

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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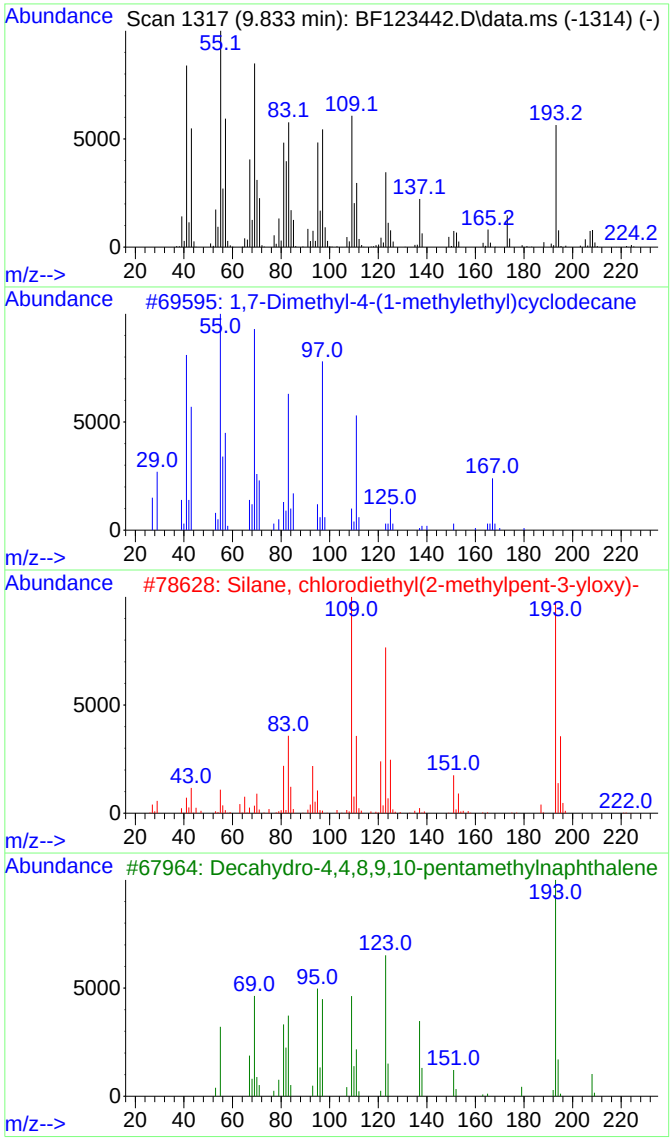
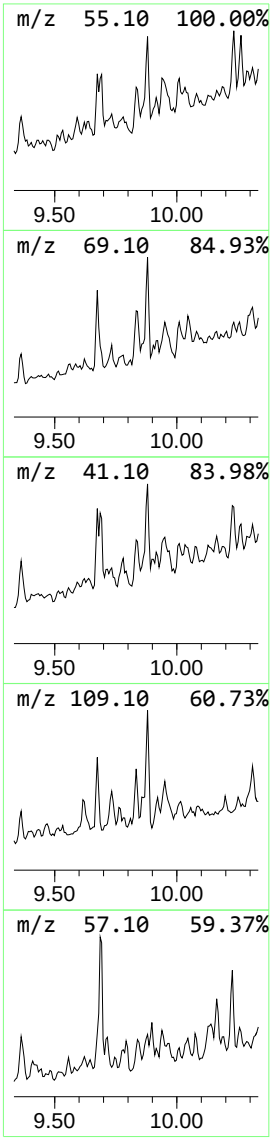
Peak Number 5 unknown9.833 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.833	9.41 ng	1813150	Acenaphthene-d10	9.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	43
2	Silane, chlorodiethyl(2-methylpe...	222	C10H23ClOSi	1000363-79-1	42
3	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	38
4	Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	30
5	Cyclopropane carboxamide, 2-cycl...	207	C13H21NO	331416-19-4	30





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

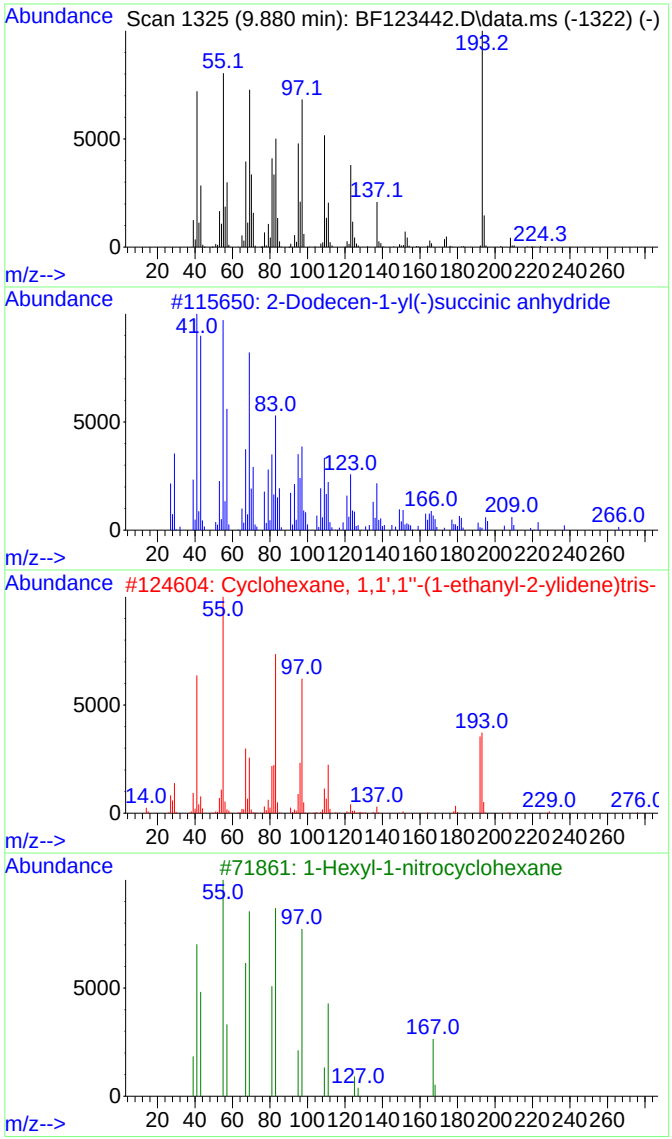
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

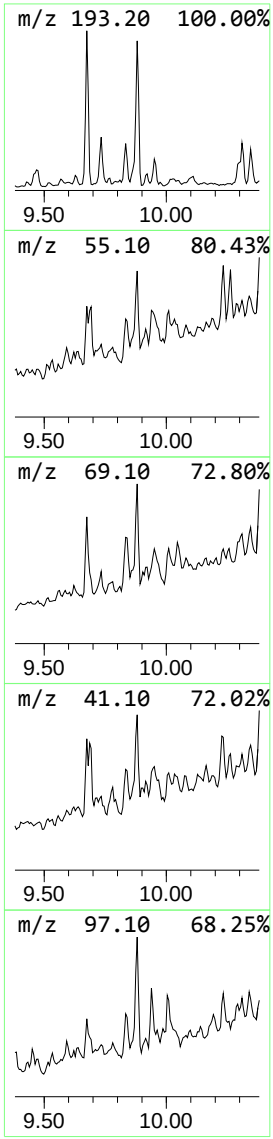
****

Peak Number 6 unknown9.880 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.880	12.04 ng	2320930	Acenaphthene-d10	9.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Dodecen-1-yl(-)succinic anhydride	266	C16H26O3	019780-11-1	43
2	Cyclohexane, 1,1',1''-(1-ethanyl...	276	C20H36	055682-86-5	38
3	1-Hexyl-1-nitrocyclohexane	213	C12H23NO2	118252-09-8	22
4	Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054823-97-1	18
5	1-Hexyl-2-nitrocyclohexane	213	C12H23NO2	118252-04-3	14





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Data File : BF123442.D
Acq On : 24 Mar 2021 16:46
Operator : JU/CG
Sample : M1777-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 248-250

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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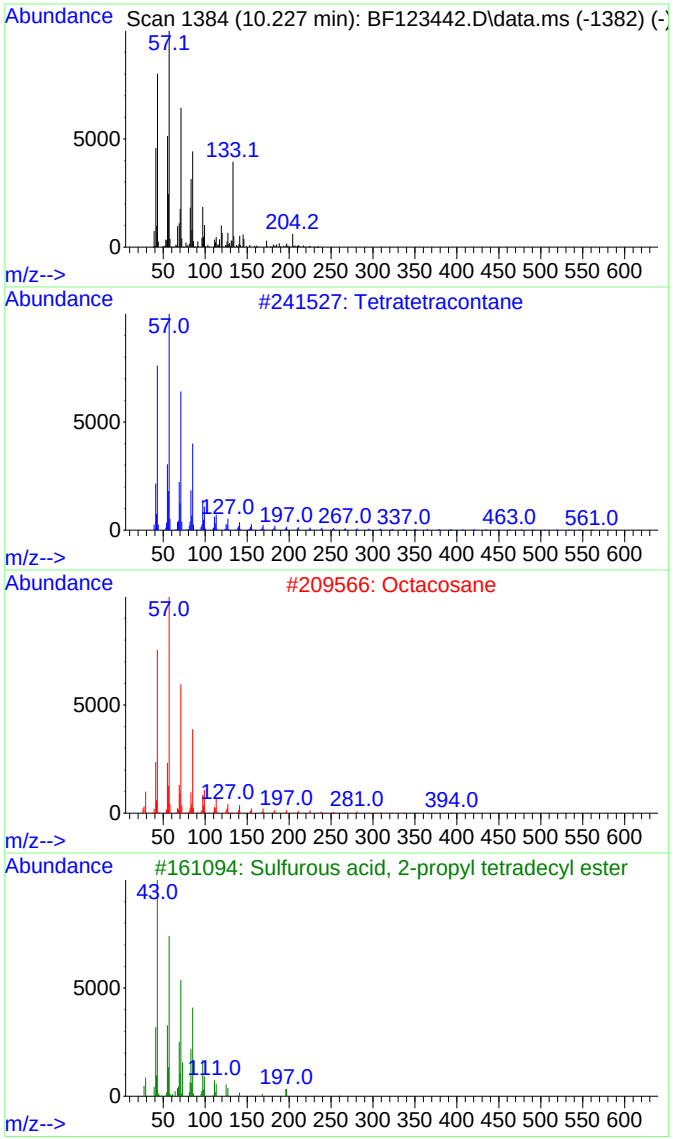
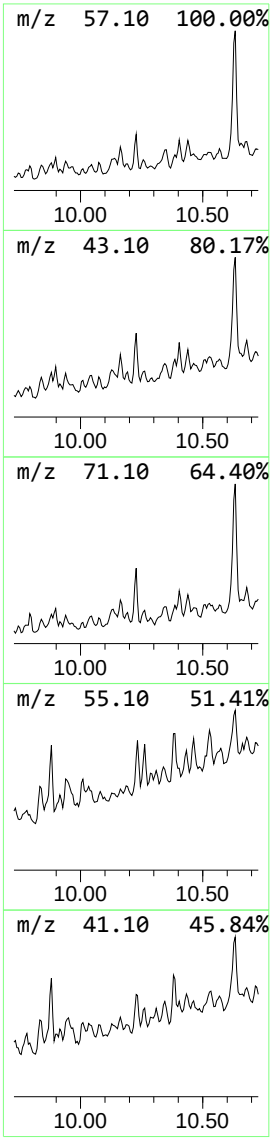
Peak Number 7 Tetratetracontane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.227	7.29 ng	1405260	Acenaphthene-d10	9.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	58
2	Octacosane	394	C28H58	000630-02-4	49
3	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	49
4	Tetracosane	338	C24H50	000646-31-1	46
5	Pentadecane	212	C15H32	000629-62-9	46





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Operator : JU/CG
Sample : M1777-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 248-250

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

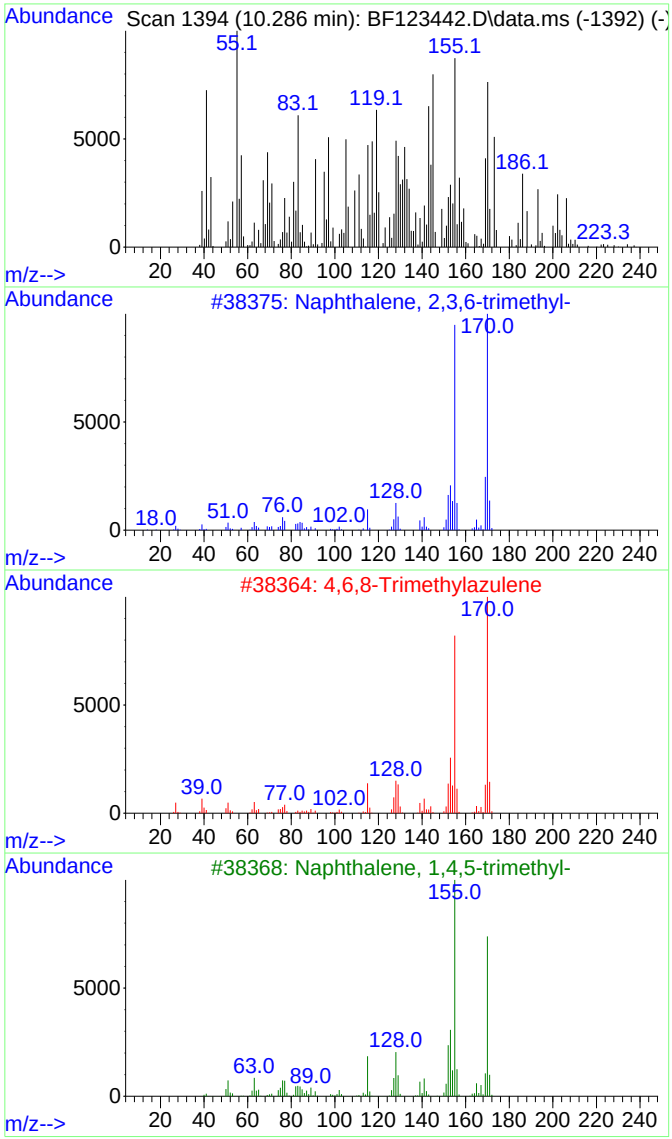
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

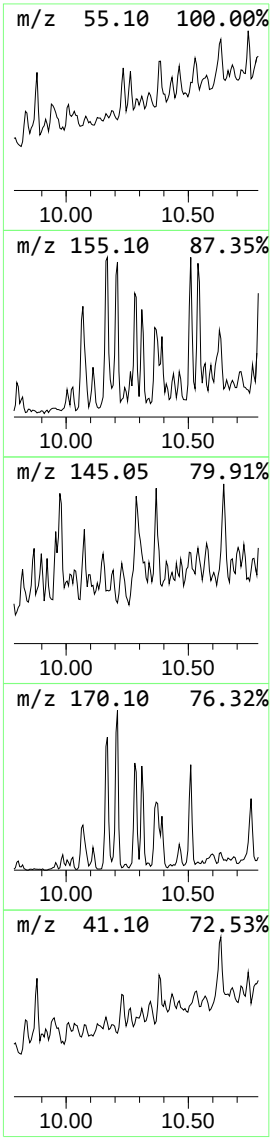
****

Peak Number 8 unknown10.286 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.286	4.59 ng	885329	Acenaphthene-d10	9.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	47
2	4,6,8-Trimethylazulene	170	C13H14	000941-81-1	38
3	Naphthalene, 1,4,5-trimethyl-	170	C13H14	002131-41-1	38
4	Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	38
5	Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	38





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Acq On : 24 Mar 2021 16:46
Operator : JU/CG
Sample : M1777-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 248-250

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

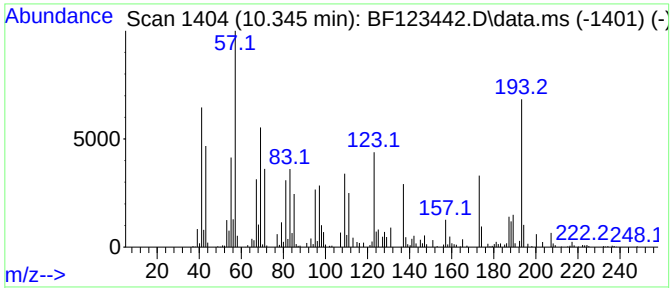
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

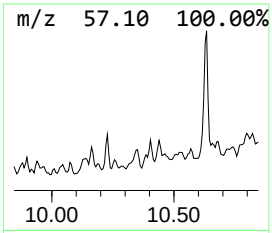
****

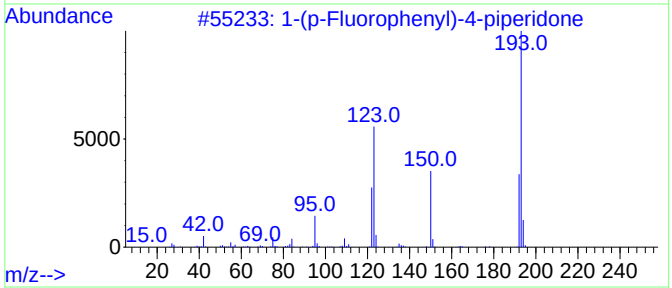
Peak Number 9 unknown10.345 Concentration Rank 18

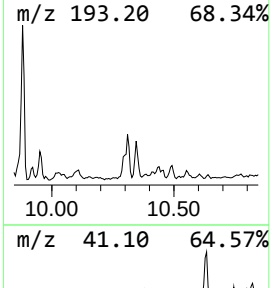
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.345	4.71 ng	908613	Acenaphthene-d10	9.963

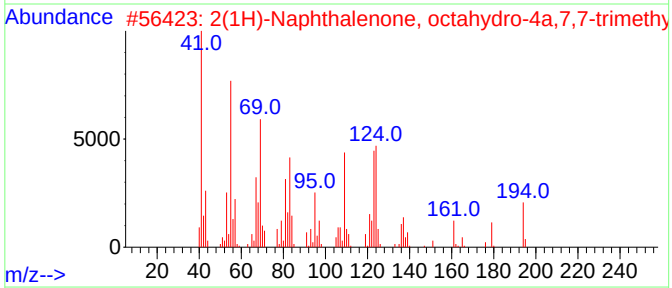
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38
2	2(1H)-Naphthalenone, octahydro-4...	194	C13H22O	007056-56-6	27
3	Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	16
4	2-Anthracenamine	193	C14H11N	000613-13-8	14
5	2,2-Dimethylpropanoic acid, 2,7-...	236	C15H24O2	1000299-33-5	14

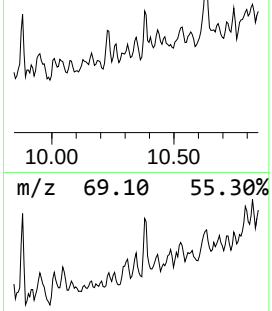


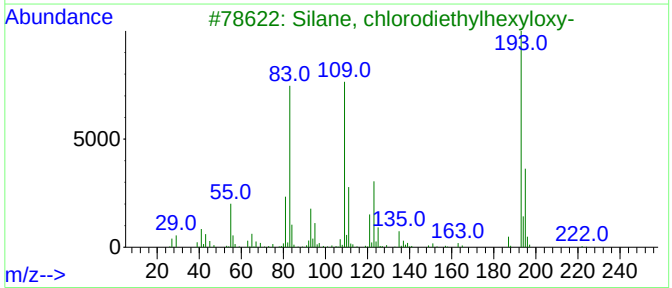












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Acq On : 24 Mar 2021 16:46
Operator : JU/CG
Sample : M1777-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 248-250

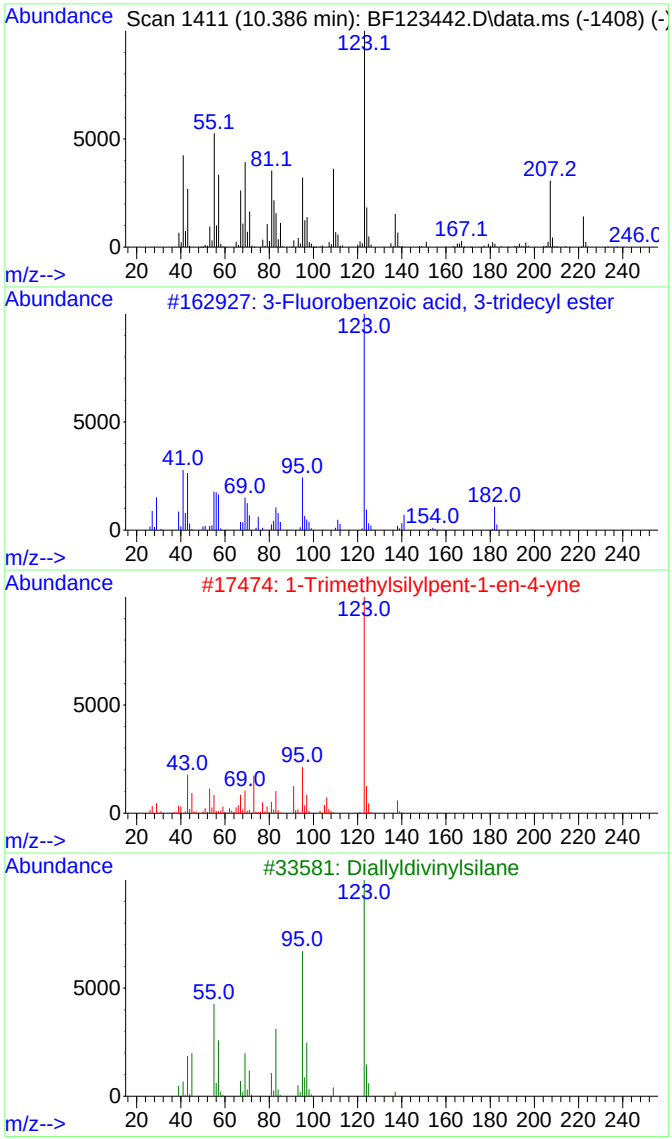
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

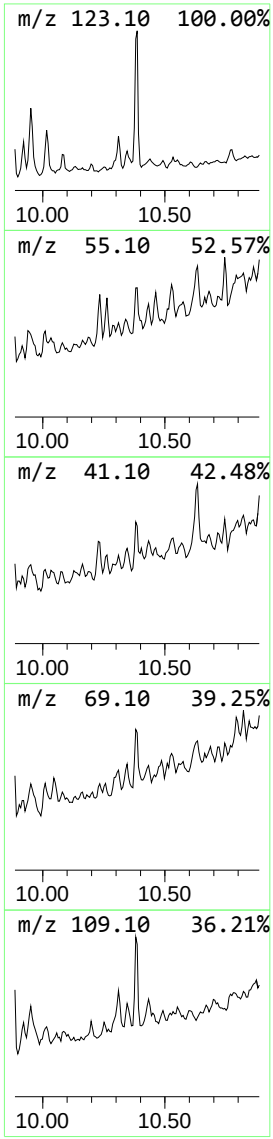
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 3-Fluorobenzoic acid, 3-tri... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.386	8.35 ng	1610180	Acenaphthene-d10	9.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Fluorobenzoic acid, 3-tridecyl...	322	C20H31FO2	1000280-60-3	50
2	1-Trimethylsilylpent-1-en-4-yne	138	C8H14Si	079516-25-9	50
3	Diallyldivinylsilane	164	C10H16Si	119901-88-1	50
4	4-Fluorobenzoic acid, 3-pentadec...	350	C22H35FO2	1000280-68-4	47
5	4-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	1000299-15-1	46





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Operator : JU/CG
Sample : M1777-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 248-250

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

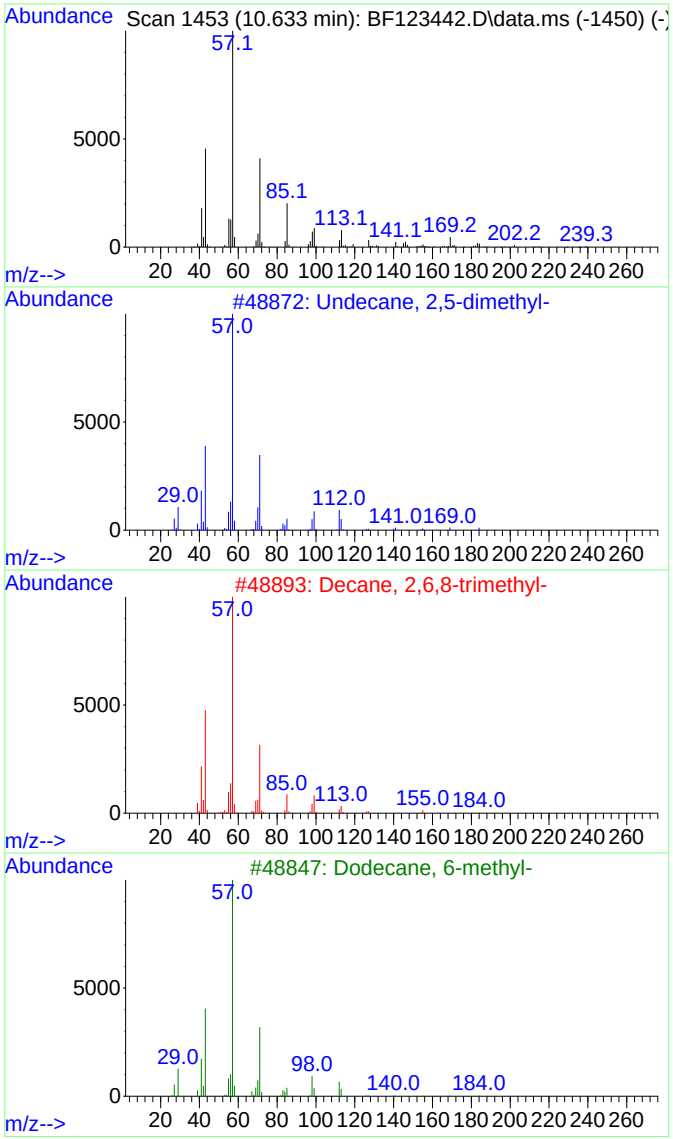
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

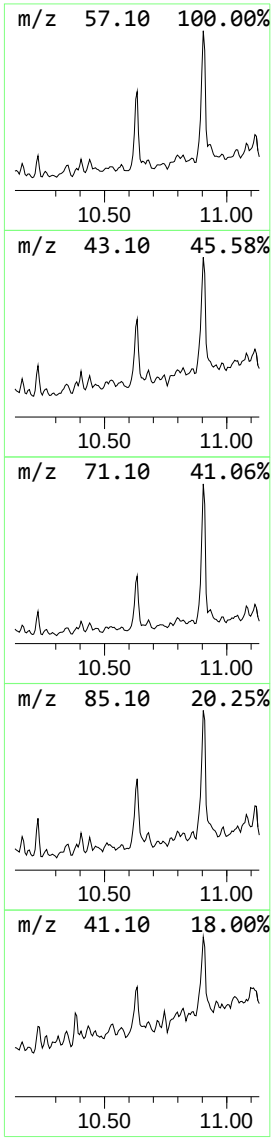
****

Peak Number 11 Undecane, 2,5-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.633	14.35 ng	2766050	Acenaphthene-d10	9.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	81
2	Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	74
3	Dodecane, 6-methyl-	184	C13H28	006044-71-9	64
4	Decane, 2-methyl-	156	C11H24	006975-98-0	64
5	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	64





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Acq On : 24 Mar 2021 16:46
Operator : JU/CG
Sample : M1777-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 248-250

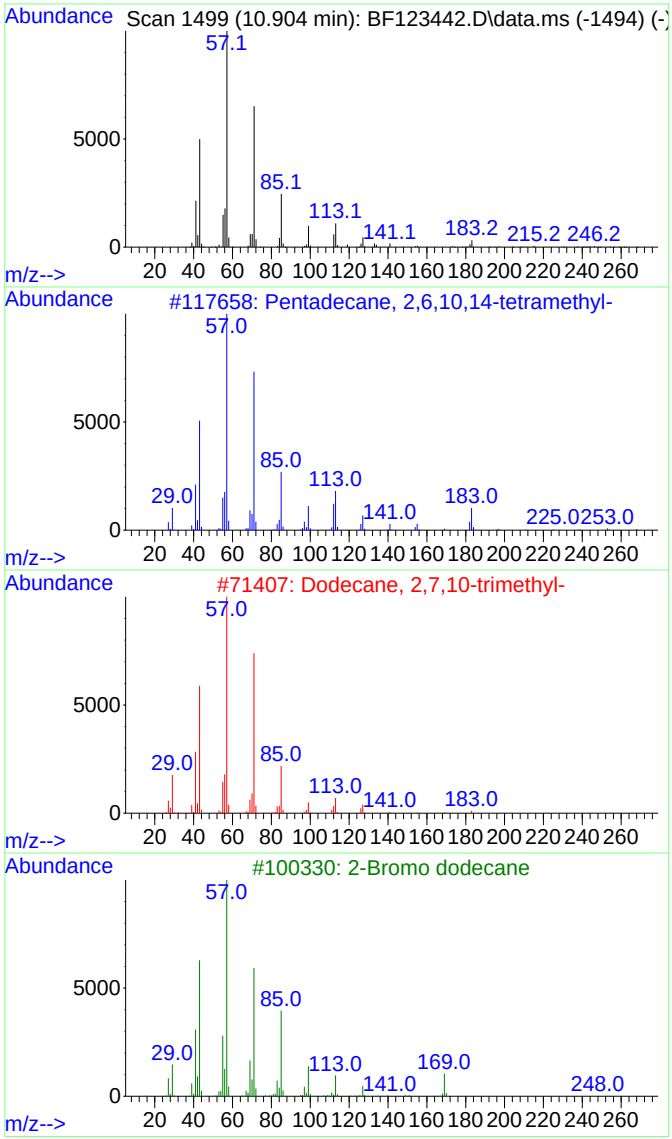
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

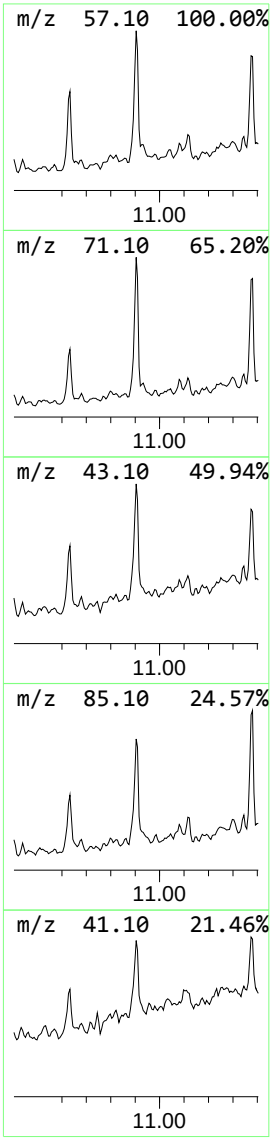
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Pentadecane, 2,6,10,14-tetr... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.904	32.53 ng	8209460	Phenanthrene-d10	11.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	91
2	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	90
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	72
4	Tridecane, 5-propyl-	226	C16H34	055045-11-9	64
5	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	59





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Operator : JU/CG
Sample : M1777-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 248-250

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

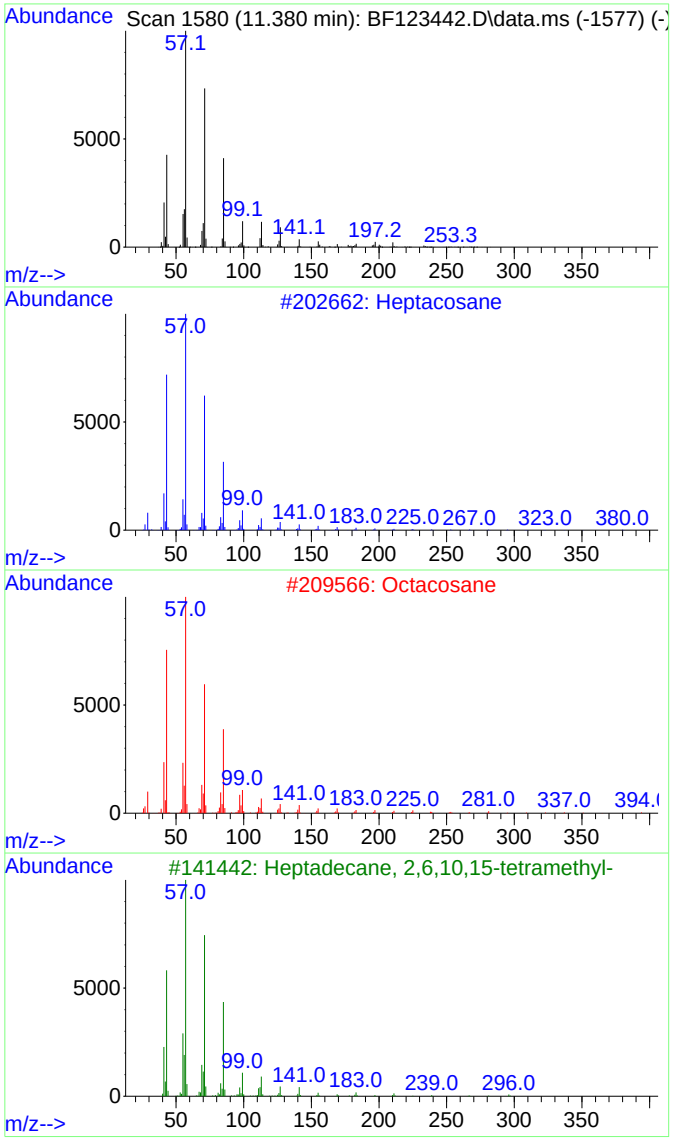
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

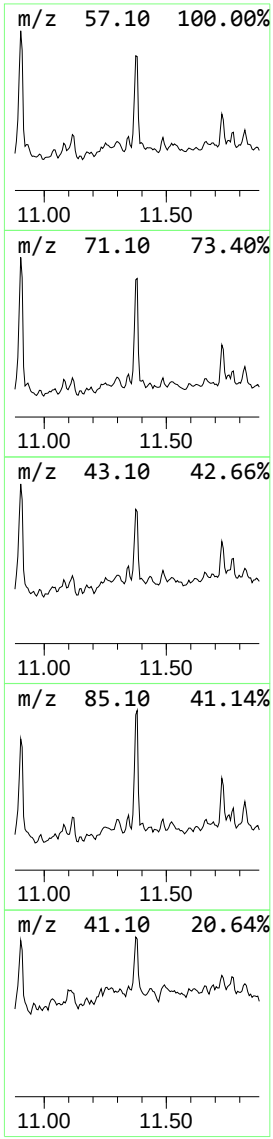
****

Peak Number 13 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.380	20.00 ng	5047140	Phenanthrene-d10	11.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	86
2	Octacosane	394	C28H58	000630-02-4	86
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
4	Tritetracontane	605	C43H88	007098-21-7	83
5	Tridecane, 2-methyl-	198	C14H30	001560-96-9	78





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Operator : JU/CG
Sample : M1777-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 248-250

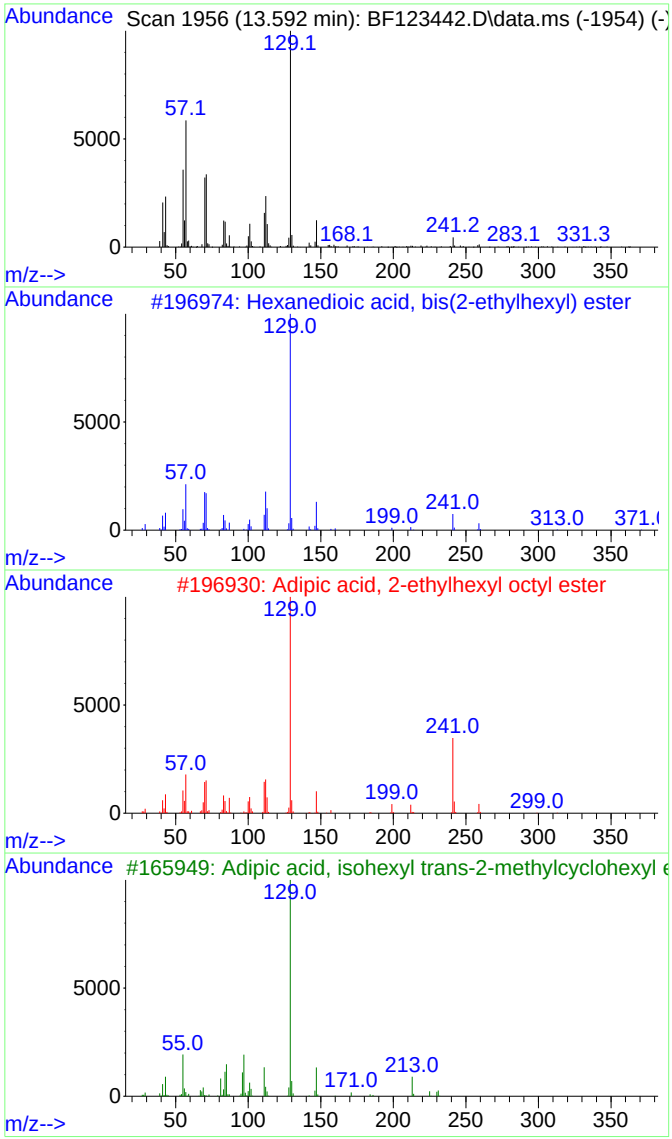
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

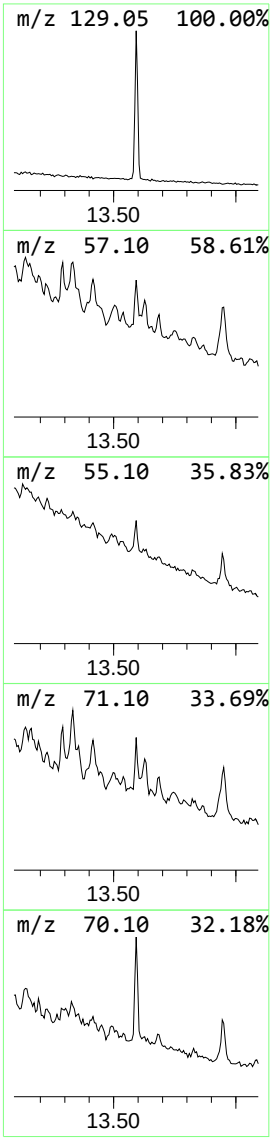
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Hexanedioic acid, bis(2-eth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.592	14.98 ng	672761	Chrysene-d12	14.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	91
2	Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	64
3	Adipic acid, isohexyl trans-2-me...	326	C19H34O4	1000324-74-8	50
4	Adipic acid, 2-methylpent-3-yl u...	384	C23H44O4	1000353-56-6	50
5	Adipic acid, cycloheptyl isohexy...	326	C19H34O4	1000324-71-8	50





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Operator : JU/CG
Sample : M1777-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 248-250

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

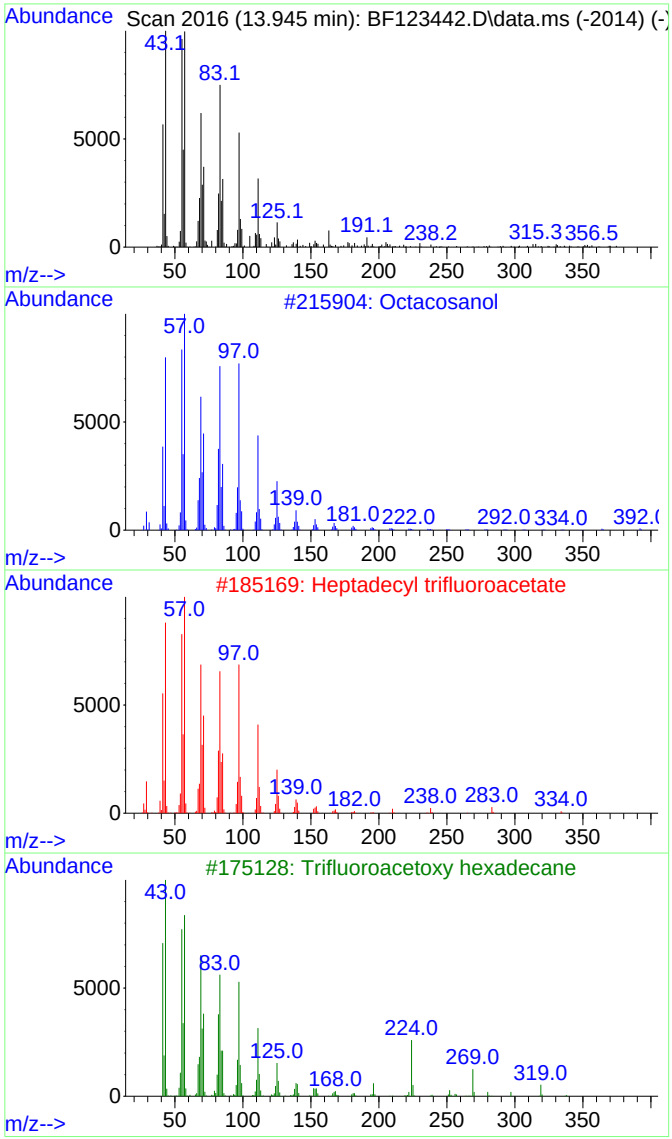
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

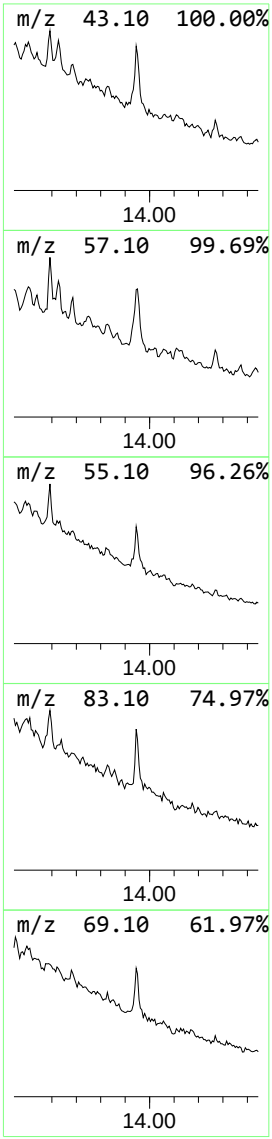
****

Peak Number 15 Octacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	31.49 ng	1414860	Chrysene-d12	14.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	90
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	90
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	86
4	Cyclotetracosane	336	C24H48	000297-03-0	86
5	1-Heptacosanol	396	C27H56O	002004-39-9	83





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Sample : M1777-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 248-250

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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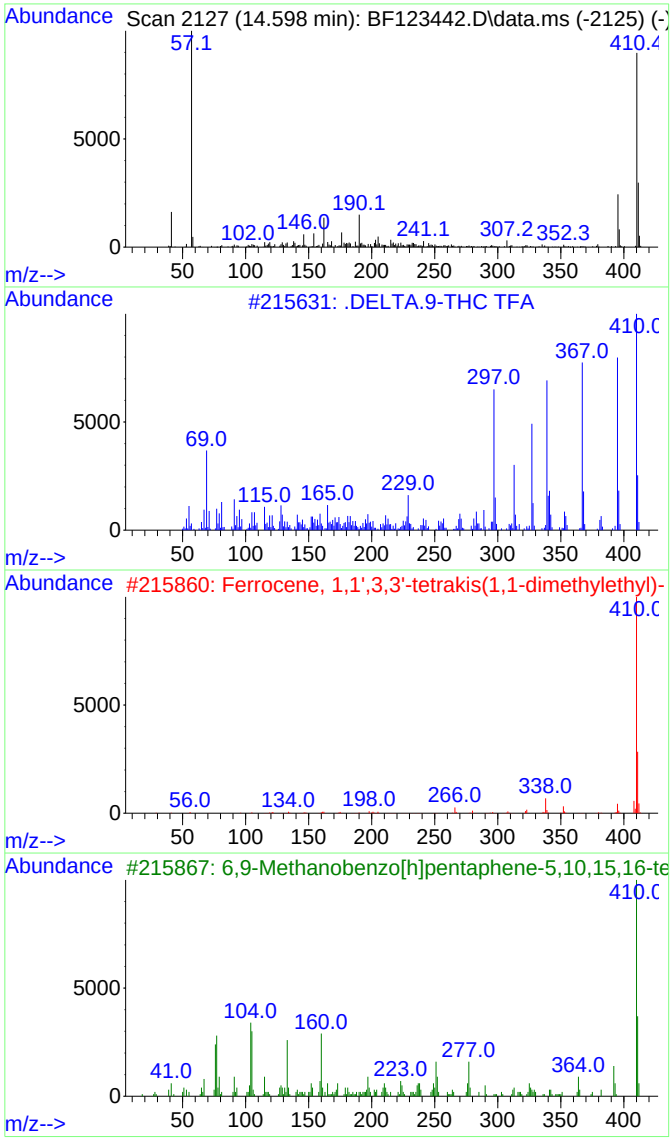
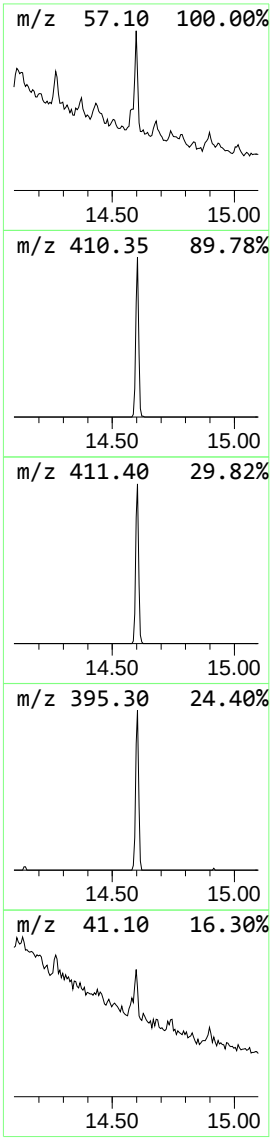
Peak Number 16 .DELTA.9-THC TFA Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.598	9.66 ng	433759	Chrysene-d12	14.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.DELTA.9-THC TFA	410	C23H29F3O3	086702-79-6	70
2	Ferrocene, 1,1',3,3'-tetrakis(1,...	410	C26H42Fe	001317-17-5	50
3	6,9-Methanobenzo[h]pentaphene-5,...	410	C27H22O4	057427-50-6	47
4	Stigmasta-4,6,22-trien-3.alpha.-ol	410	C29H46O	1000103-93-1	38
5	3-Acetyl-1-(3,4-dimethoxyphenyl)...	410	C23H26N2O5	090140-65-1	28





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Sample : M1777-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
248-250

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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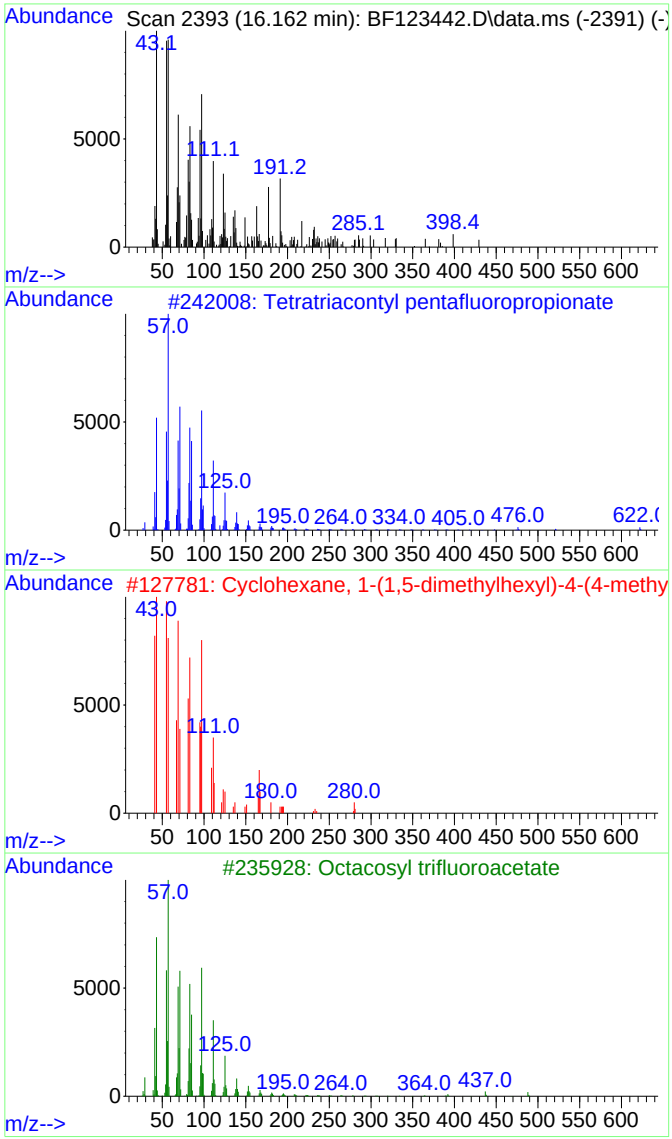
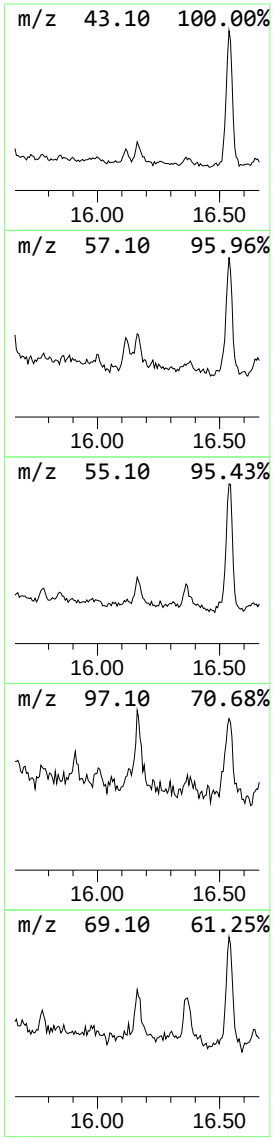
Peak Number 17 unknown16.162 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.162	6.61 ng	364117	Perylene-d12	15.609

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	43
2	Cyclohexane, 1-(1,5-dimethylhexy...	280	C20H40	056009-20-2	43
3	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	43
4	Cyclooctadecane, ethyl-	280	C20H40	1000151-22-5	42
5	1-Octadecanethiol	286	C18H38S	002885-00-9	35





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Acq On : 24 Mar 2021 16:46
Operator : JU/CG
Sample : M1777-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 248-250

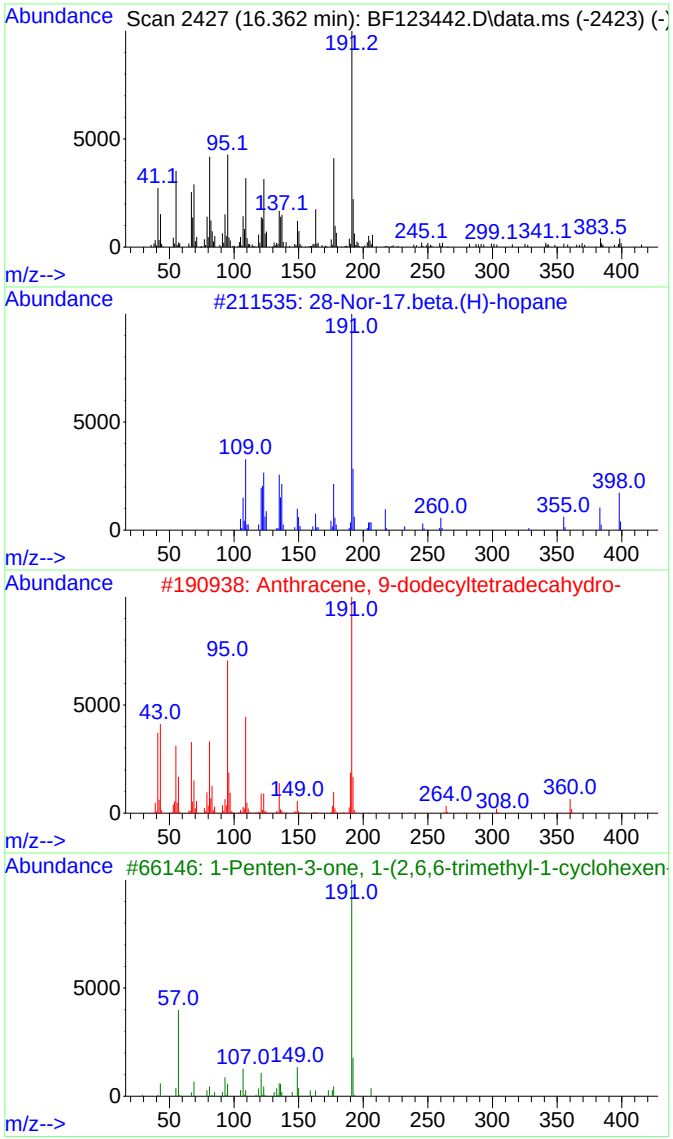
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

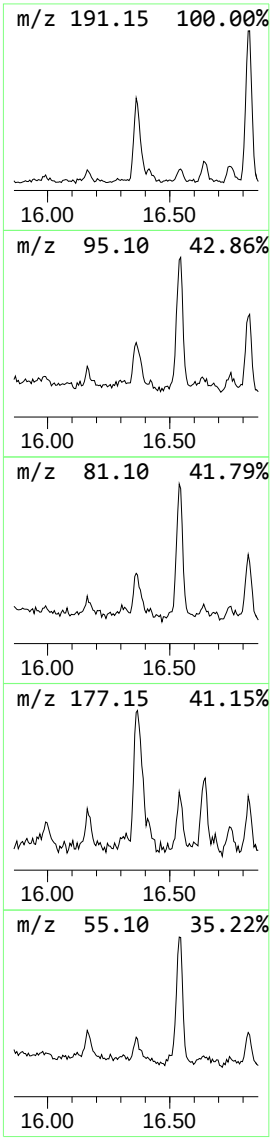
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 28-Nor-17.beta.(H)-hopane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.362	9.06 ng	499051	Perylene-d12	15.609

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	76
2	Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	40
3	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	35
4	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	32
5	Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	27





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Data File : BF123442.D
Acq On : 24 Mar 2021 16:46
Operator : JU/CG
Sample : M1777-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 248-250

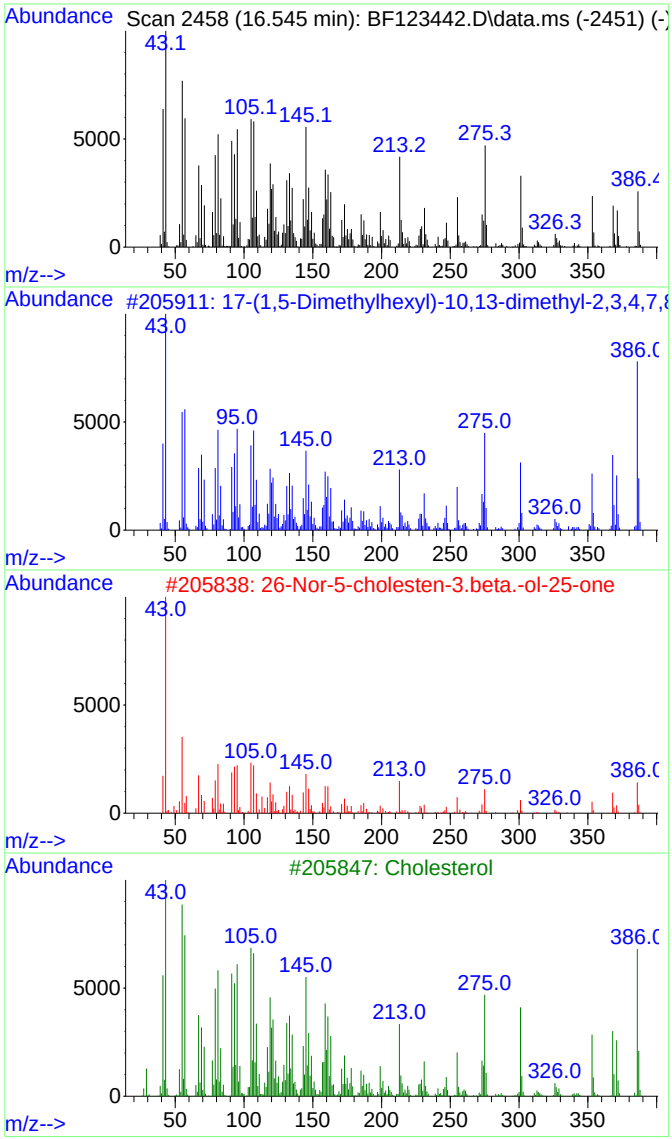
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

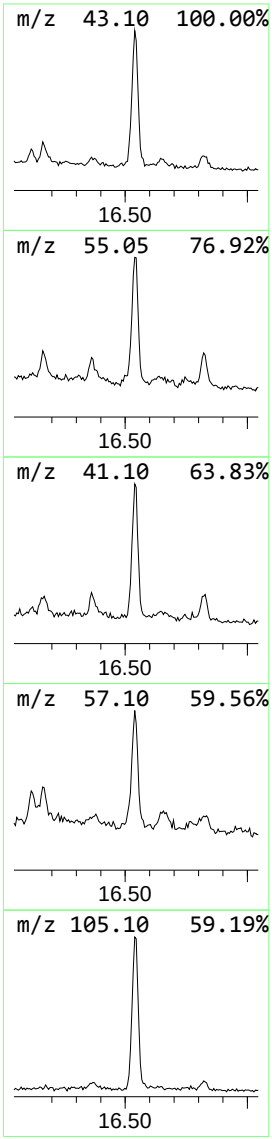
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 17-(1,5-Dimethylhexyl)-10,1... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.545	58.17 ng	3203370	Perylene-d12	15.609

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-(1,5-Dimethylhexyl)-10,13-dim...	386	C27H46O	1000210-38-4	99
2	26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	99
3	Cholesterol	386	C27H46O	000057-88-5	98
4	Cholestane-3,5-diol, 5-acetate, ...	446	C29H50O3	041721-93-1	43
5	Cholesta-3,5-diene	368	C27H44	000747-90-0	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
Data File : BF123442.D
Acq On : 24 Mar 2021 16:46
Operator : JU/CG
Sample : M1777-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 248-250

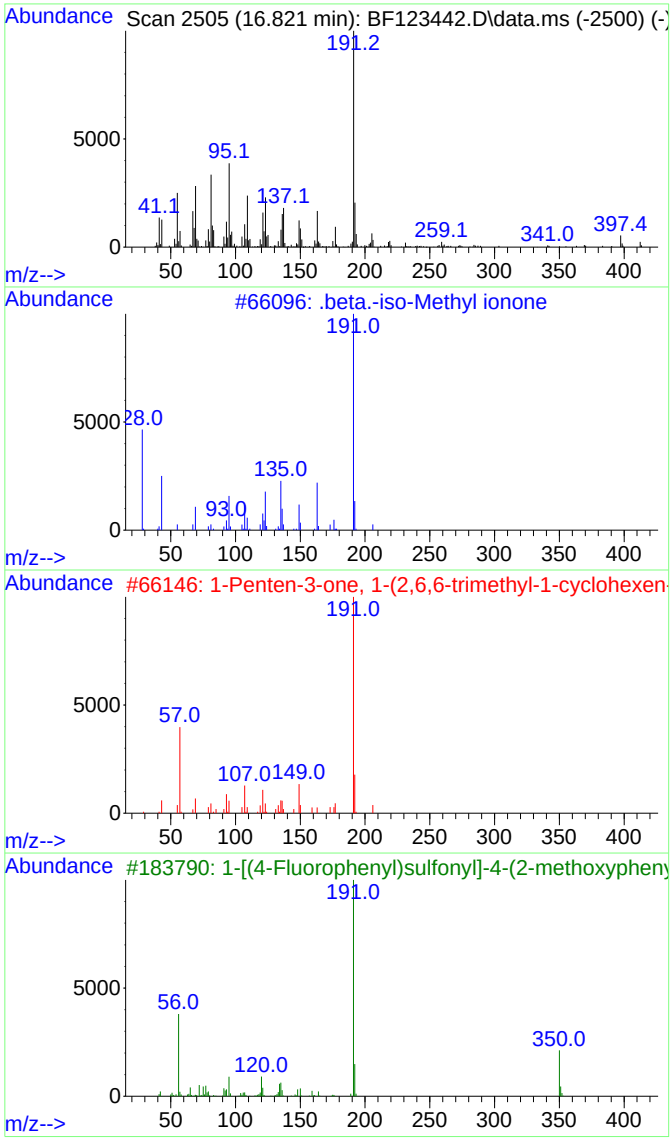
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

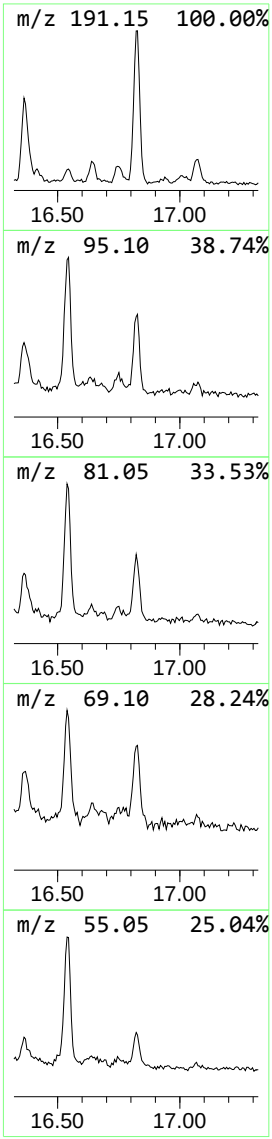
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 .beta.-iso-Methyl ionone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.821	14.50 ng	798568	Perylene-d12	15.609

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	74
2	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	43
3	1-[(4-Fluorophenyl)sulfonyl]-4-(...	350	C17H19FN2O3S	260554-69-6	35
4	3-Fluoro-5-trifluoromethylbenzoi...	376	C20H28F4O2	1000338-65-7	35
5	4-Fluoro-3-trifluoromethylbenzoi...	376	C20H28F4O2	1000338-67-4	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
Data File : BF123442.D
Acq On : 24 Mar 2021 16:46
Operator : JU/CG
Sample : M1777-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 248-250

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.228	24.8	ng	1593670	1	6.916	1284260	20.0
Dodecane, 2,6,1...	9.227	4.4	ng	844388	3	9.963	3854950	20.0
unknown9.363	9.363	9.7	ng	1873150	3	9.963	3854950	20.0
2,5-Cyclohexadi...	9.780	7.0	ng	1343410	3	9.963	3854950	20.0
unknown9.833	9.833	9.4	ng	1813150	3	9.963	3854950	20.0
unknown9.880	9.880	12.0	ng	2320930	3	9.963	3854950	20.0
Tetratetracontane	10.227	7.3	ng	1405260	3	9.963	3854950	20.0
unknown10.286	10.286	4.6	ng	885329	3	9.963	3854950	20.0
unknown10.345	10.345	4.7	ng	908613	3	9.963	3854950	20.0
3-Fluorobenzoic...	10.386	8.3	ng	1610180	3	9.963	3854950	20.0
Undecane, 2,5-d...	10.633	14.4	ng	2766050	3	9.963	3854950	20.0
Pentadecane, 2,...	10.904	32.5	ng	8209460	4	11.469	5047140	20.0
Heptacosane	11.380	20.0	ng	5047140	4	11.469	5047140	20.0
Hexanedioic aci...	13.592	15.0	ng	672761	5	14.110	898491	20.0
Octacosanol	13.945	31.5	ng	1414860	5	14.110	898491	20.0
.DELTA.9-THC TFA	14.598	9.7	ng	433759	5	14.110	898491	20.0
unknown16.162	16.162	6.6	ng	364117	6	15.609	1101410	20.0
28-Nor-17.beta....	16.362	9.1	ng	499051	6	15.609	1101410	20.0
17-(1,5-Dimethy...	16.545	58.2	ng	3203370	6	15.609	1101410	20.0
.beta.-iso-Meth...	16.821	14.5	ng	798568	6	15.609	1101410	20.0