LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
Data File : BF133184.D
Acq On : 02 May 2023 12:42
Operator : CG\JU
Sample : 02521-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-15

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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

Signal : TIC: BF133184.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.010	492	497	501	rVB	514007	532371	9.16%	1.355%
2	5.340	549	553	556	rBV	2897624	2545238	43.77%	6.477%
3	6.363	723	727	730	rBV	2077321	1640714	28.22%	4.175%
4	6.669	774	779	781	rBV	59117	65701	1.13%	0.167%
5	6.728	785	789	792	rBV	1557134	1253207	21.55%	3.189%
6	6.893	811	817	818	rBV	78056	69024	1.19%	0.176%
7	6.910	818	820	824	rVB	227624	169806	2.92%	0.432%
8	6.981	830	832	835	rBV	108293	76838	1.32%	0.196%
9	7.075	846	848	854	rVB2	84522	74495	1.28%	0.190%
10	7.298	875	886	889	rBV	3617014	3844799	66.12%	9.784%
11	7.375	895	899	903	rBV3	75714	84625	1.46%	0.215%
12	7.422	903	907	909	rVV2	61166	79869	1.37%	0.203%
13	7.451	909	912	915	rVV	751160	574497	9.88%	1.462%
14	7.504	919	921	924	rVB	221792	158737	2.73%	0.404%
15	7.622	938	941	944	rVB2	109418	99624	1.71%	0.254%
16	7.669	944	949	951	rBV2	78844	95016	1.63%	0.242%
17	7.757	958	964	966	rBV2	187899	186352	3.20%	0.474%
18	7.922	987	992	997	rBV7	56554	109456	1.88%	0.279%
19	7.975	997	1001	1003	rVV	123299	103346	1.78%	0.263%
20	8.010	1004	1007	1010	rVB	1923636	1640140	28.21%	4.174%
21	8.340	1059	1063	1066	rBV	183602	157073	2.70%	0.400%
22	8.392	1069	1072	1075	rVB3	86775	90716	1.56%	0.231%
23	8.481	1083	1087	1092	rVB6	43946	65053	1.12%	0.166%
24	8.540	1092	1097	1099	rBV4	60684	86338	1.48%	0.220%
25	8.587	1102	1105	1109	rVV	213702	224706	3.86%	0.572%
26	8.640	1112	1114	1118	rVB3	89264	106761	1.84%	0.272%
27	8.787	1135	1139	1142	rVB4	101992	115002	1.98%	0.293%
28	8.904	1155	1159	1162	rBV5	59111	83888	1.44%	0.213%
29	8.945	1162	1166	1171	rVB6	44966	87189	1.50%	0.222%
30	9.092	1186	1191	1194	rBV	6759408	5814476	100.00%	14.796%
31	9.281	1220	1223	1228	rVB7	41976	68857	1.18%	0.175%
32	9.445	1249	1251	1258	rVB4	63817	75313	1.30%	0.192%
33	9.722	1296	1298	1302	rBV2	54224	72930	1.25%	0.186%
34	9.763	1302	1305	1309	rVB	2140229	1870990	32.18%	4.761%
35	10.481	1422	1427	1430	rBV	386691	364691	6.27%	0.928%
36	10.557	1435	1440	1443	rBV	4133780	3964520	68.18%	10.088%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
Data File : BF133184.D
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Operator : CG\JU
Sample : 02521-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-15

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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

37	10.657	1454	1457	1460	rBV	294290	256718	4.42%	0.653%
38	10.839	1485	1488	1491	rBV	341740	287335	4.94%	0.731%
39	11.245	1554	1557	1561	rBV	2182313	1901771	32.71%	4.839%
40	11.786	1645	1649	1659	rBV	875346	936569	16.11%	2.383%
41	12.569	1779	1782	1789	rBV	252436	261514	4.50%	0.665%
42	12.680	1798	1801	1804	rVB	177203	136697	2.35%	0.348%
43	12.839	1823	1828	1831	rBV	5792754	5608636	96.46%	14.272%
44	13.757	1980	1984	1995	rVB3	260457	495410	8.52%	1.261%
45	13.880	2001	2005	2008	rBV	1493674	1386066	23.84%	3.527%
46	13.910	2008	2010	2014	rVB	130509	110768	1.91%	0.282%
47	14.733	2147	2150	2154	rVB	277172	253530	4.36%	0.645%
48	15.304	2242	2247	2251	rBV	894791	1011381	17.39%	2.574%

Sum of corrected areas: 39298753

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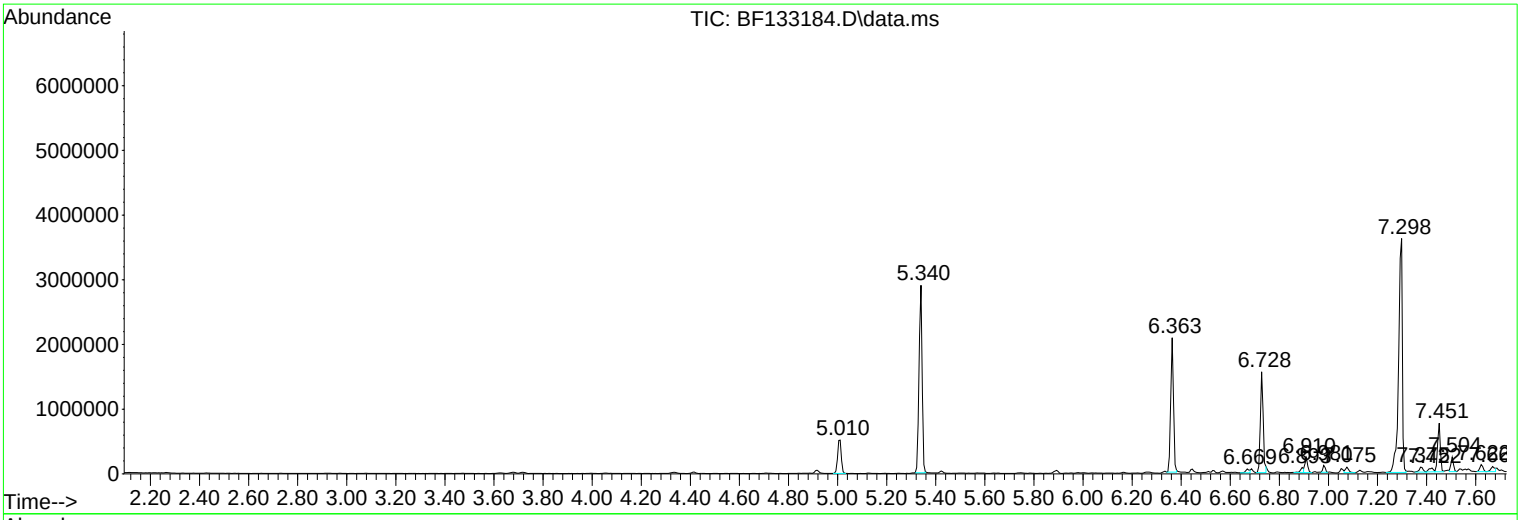
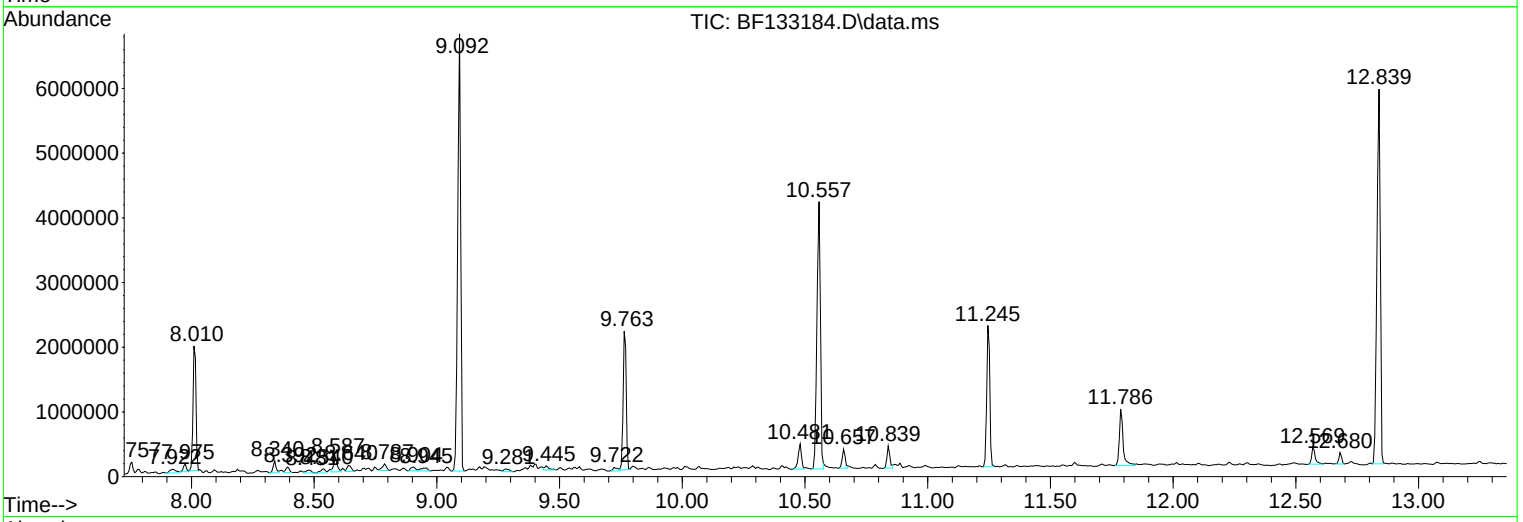
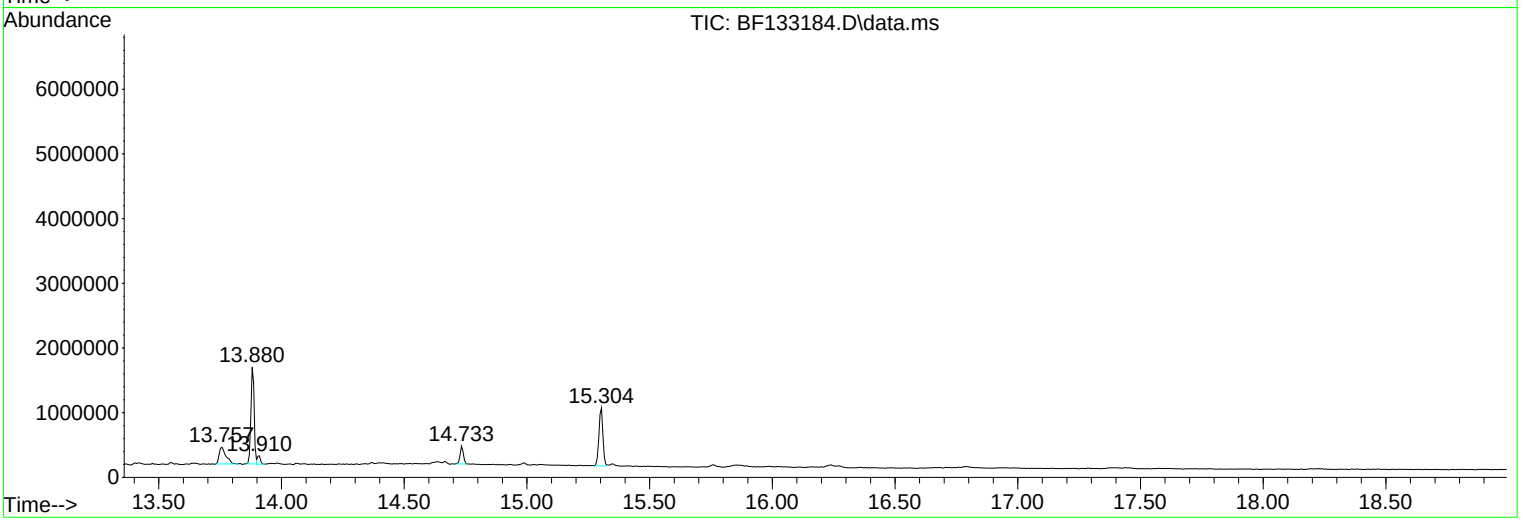
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Data File : BF133184.D
Acq On : 02 May 2023 12:42
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Sample : 02521-03
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Instrument :
BNA_F
ClientSampleId :
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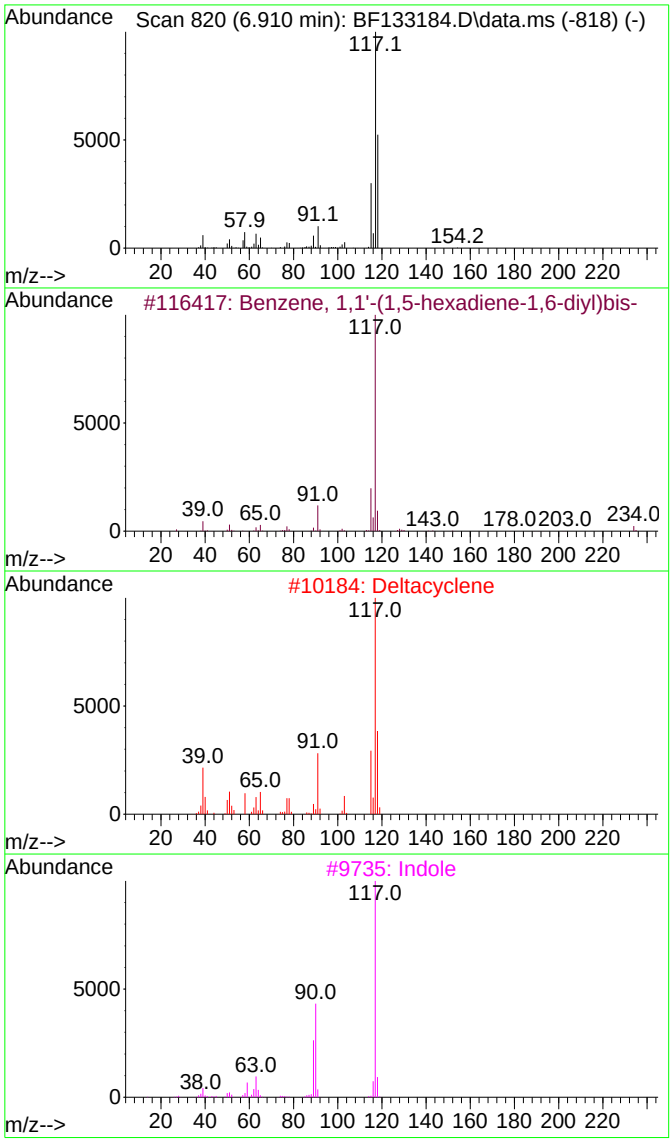
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

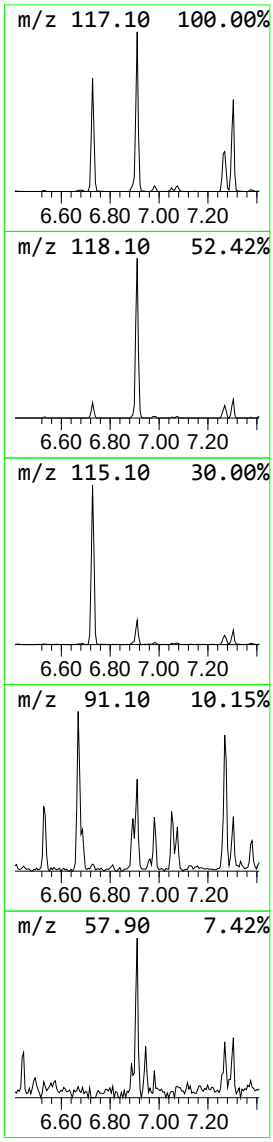
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.910	2.71 ng	169806	1,4-Dichlorobenzene-d4	6.728

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	53
2	Deltacyclene	118	C9H10	007785-10-6	50
3	Indole	117	C8H7N	000120-72-9	43
4	m-Aminophenylacetylene	117	C8H7N	054060-30-9	43
5	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	40





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Data File : BF133184.D
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Operator : CG\JU
Sample : 02521-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-15

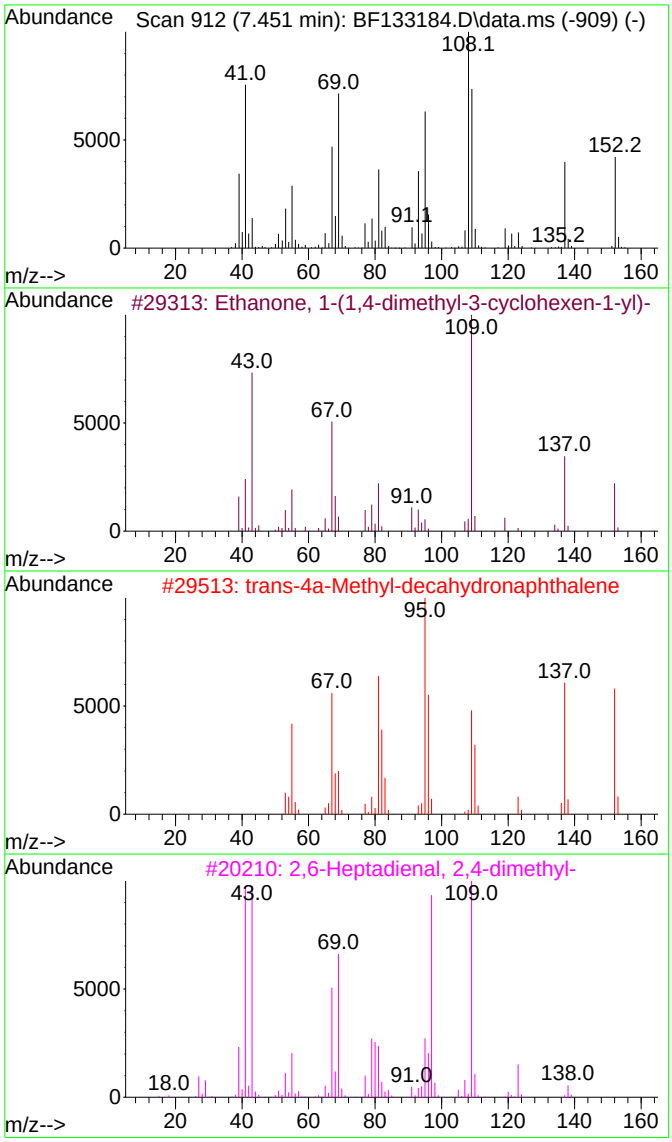
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

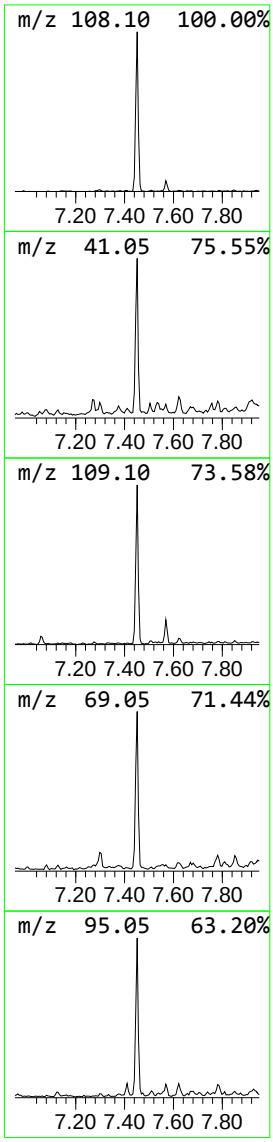
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanone, 1-(1,4-dimethyl-3... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.451	7.01 ng	574497	Naphthalene-d8	8.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(1,4-dimethyl-3-cycl...	152	C10H16O	043219-68-7	60
2	trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	45
3	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	38
4	2,3,4-Trimethylpyrrole	109	C7H11N	003855-78-5	38
5	Ethanol, 2-(3-methylphenoxy)-	152	C9H12O2	013605-19-1	30





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Data File : BF133184.D
Acq On : 02 May 2023 12:42
Operator : CG\JU
Sample : 02521-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-15

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

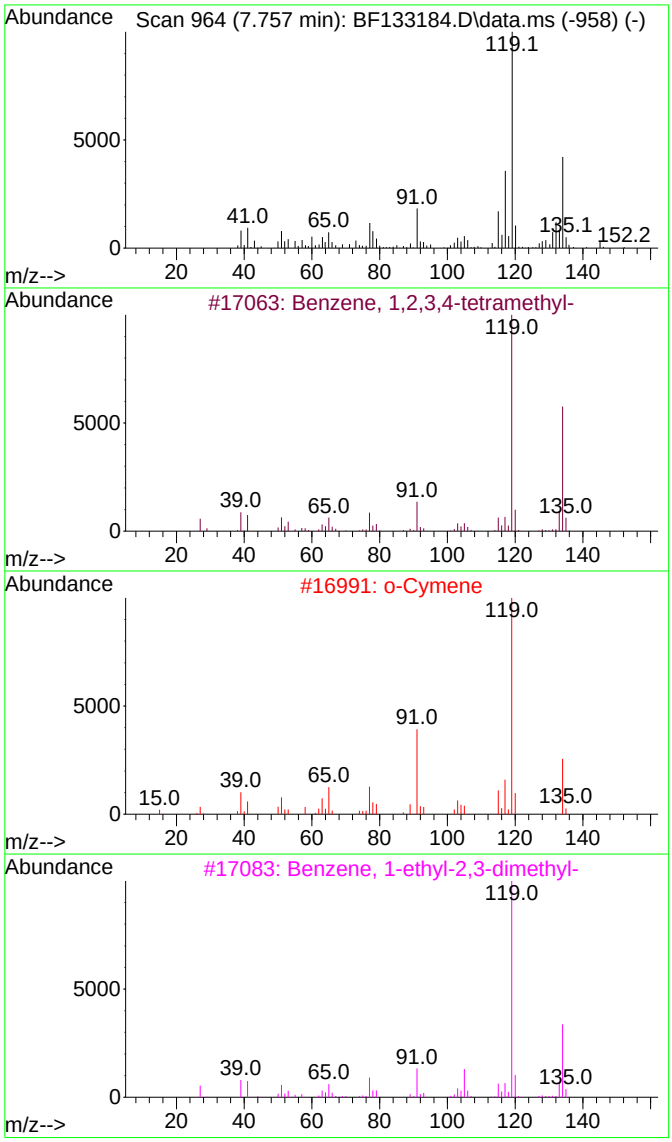
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

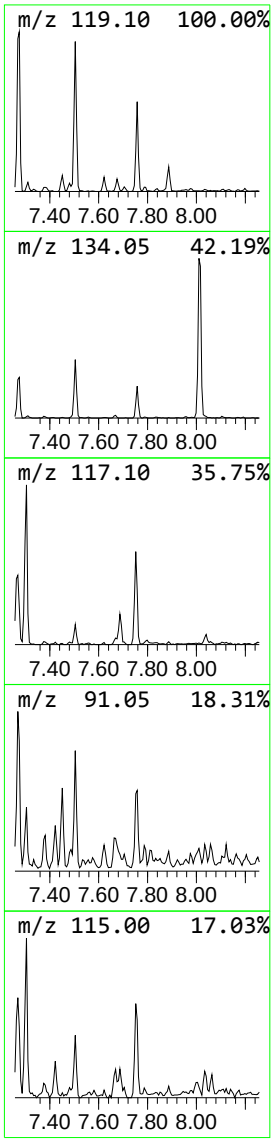
****

Peak Number 4 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.757	2.27 ng	186352	Naphthalene-d8	8.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	81
2	o-Cymene	134	C10H14	000527-84-4	81
3	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	81
4	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	81
5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	81





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Sample : 02521-03
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Instrument :
BNA_F
ClientSampleId :
PZ-15

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

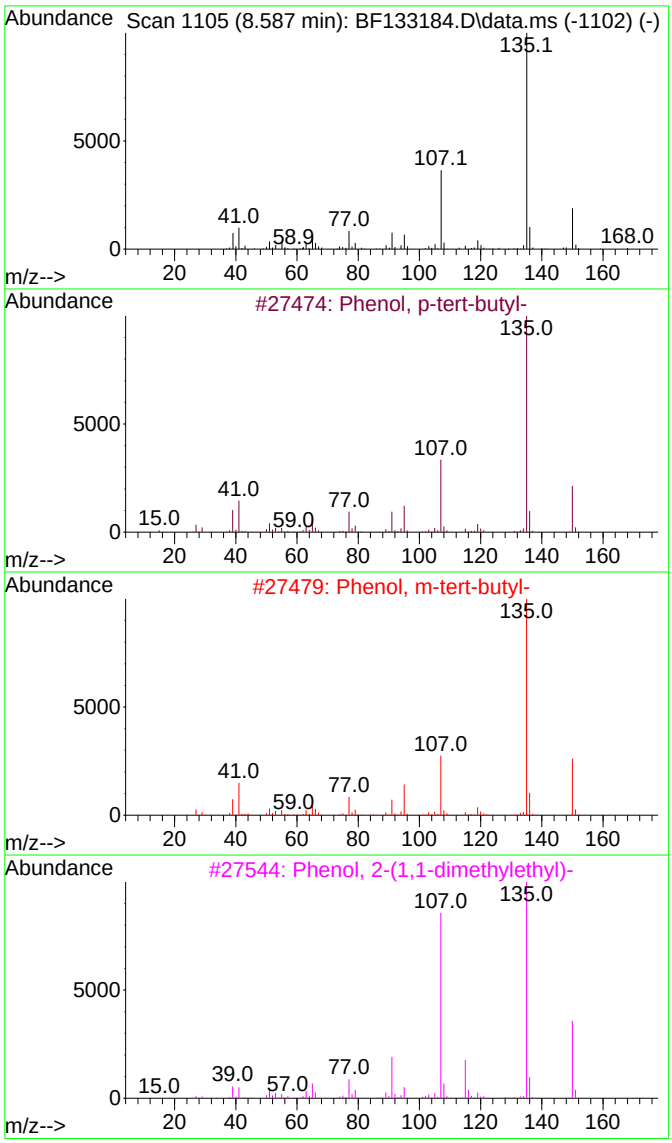
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

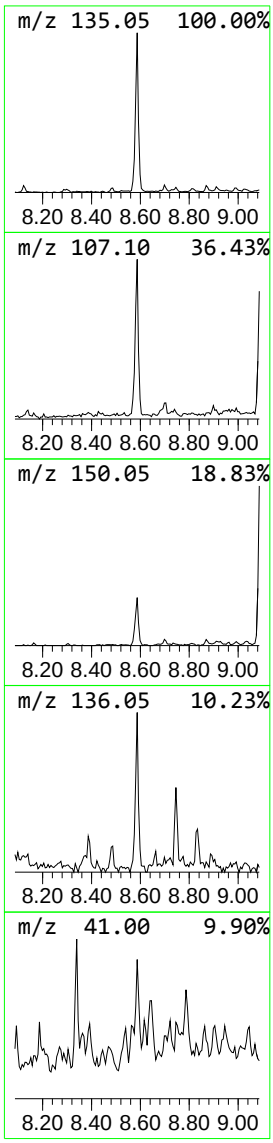
****

Peak Number 5 Phenol, p-tert-butyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.587	2.74 ng	224706	Naphthalene-d8	8.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	94
2	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	91
3	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	90
4	4,4'-(1,2-diethylethylene)diphenol	270	C18H22O2	005635-50-7	64
5	1-Propanone, 1-(3-methoxyphenyl)-	164	C10H12O2	037951-49-8	64





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

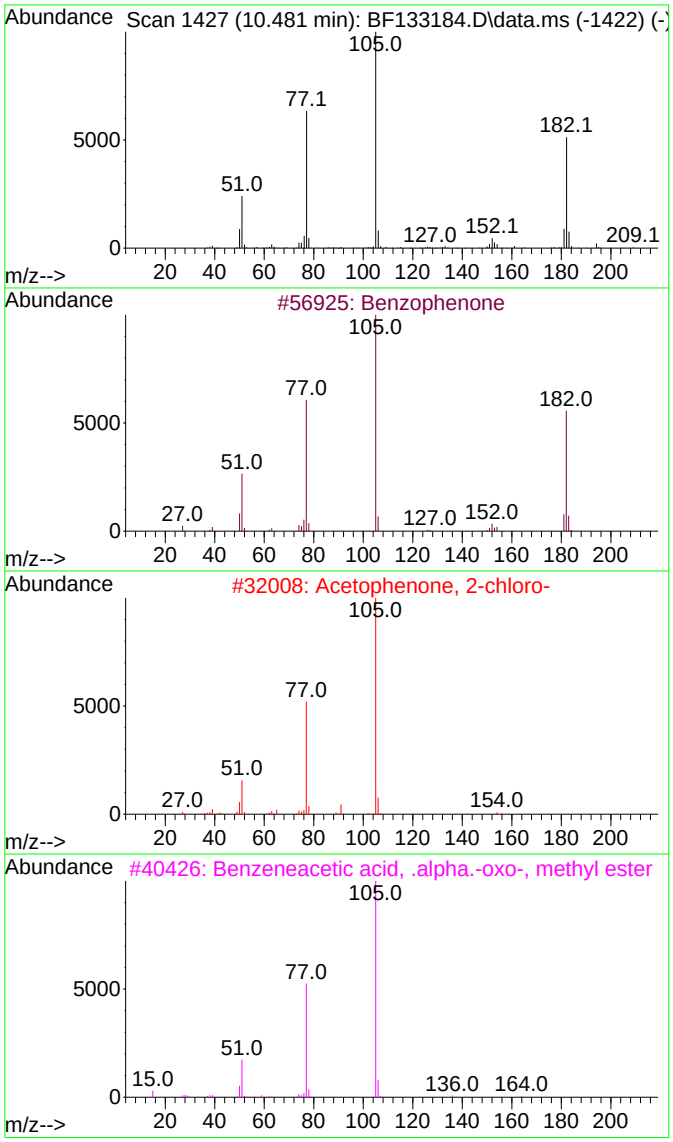
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

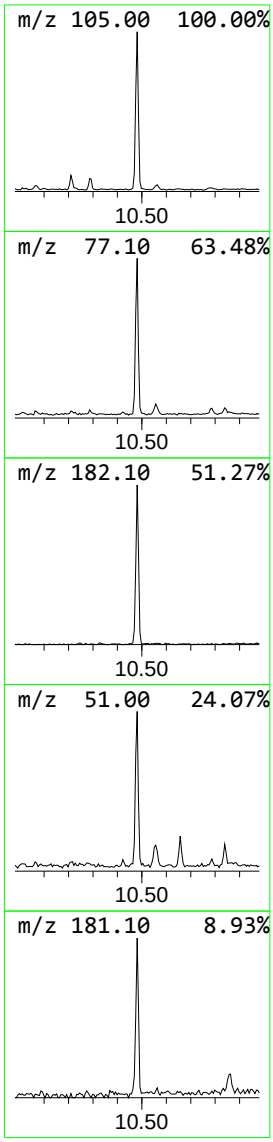
****

Peak Number 6 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.481	3.90 ng	364691	Acenaphthene-d10	9.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
3	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
4	Benzoic acid, 2-propenyl ester	162	C10H10O2	000583-04-0	47
5	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47





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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-15

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

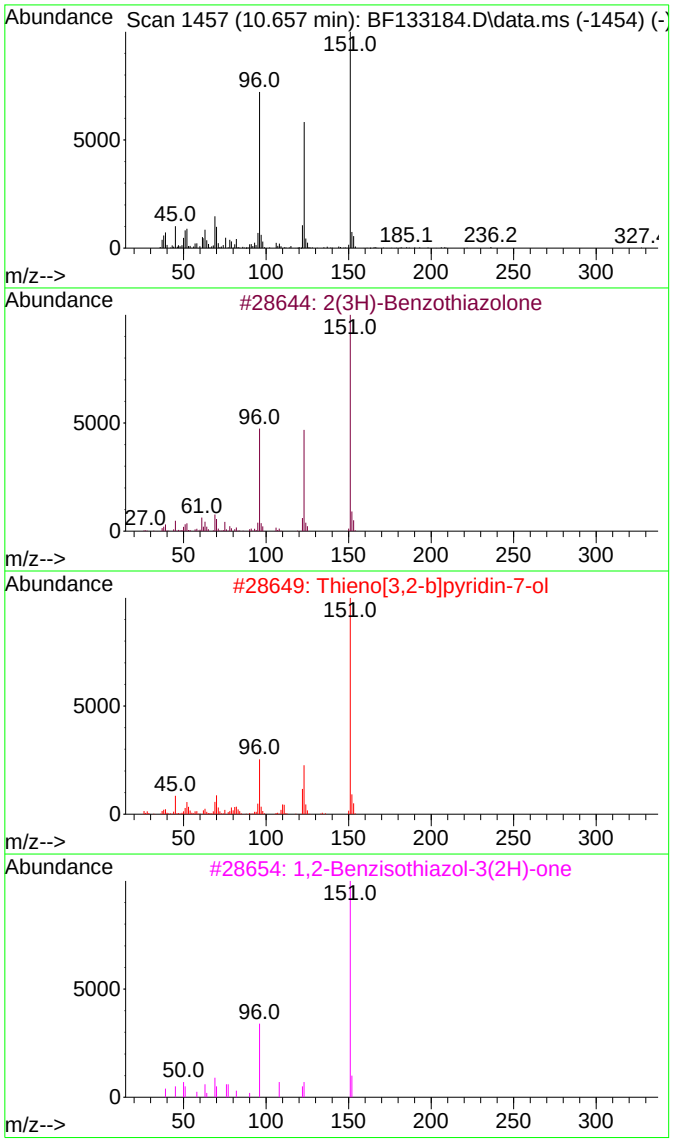
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

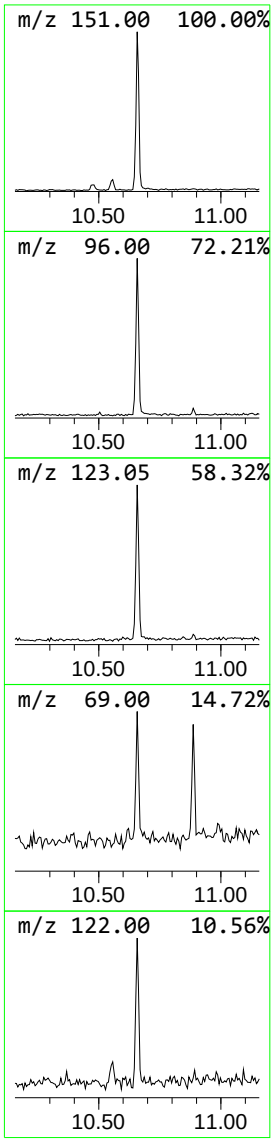
****

Peak Number 7 2(3H)-Benzothiazolone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.657	2.70 ng	256718	Phenanthrene-d10	11.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	97
2	Thieno[3,2-b]pyridin-7-ol	151	C7H5NOS	107818-20-2	58
3	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	53
4	6-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057250-39-2	50
5	4-Methoxyformanilide	151	C8H9NO2	005470-34-8	43





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

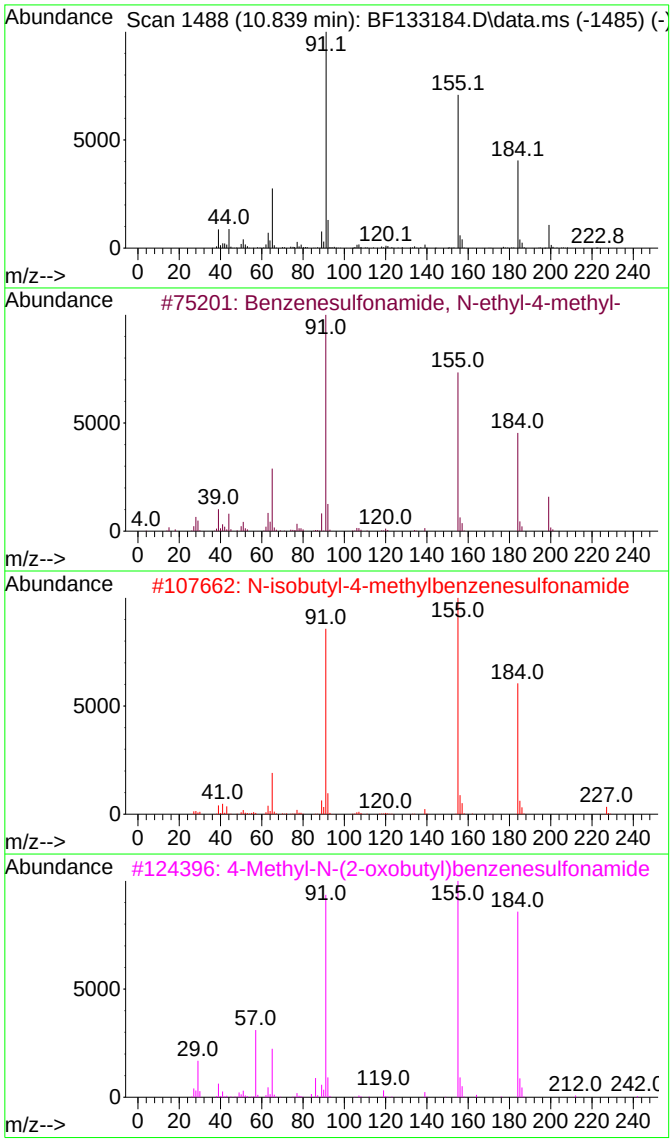
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

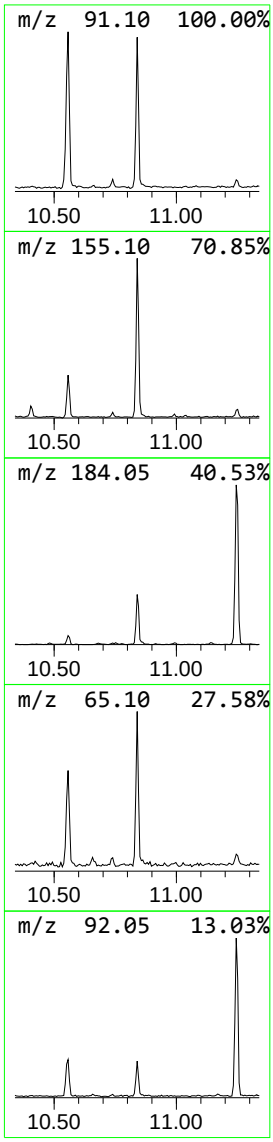
****

Peak Number 8 Benzenesulfonamide, N-ethyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.839	3.02 ng	287335	Phenanthrene-d10	11.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	98
2	N-isobutyl-4-methylbenzenesulfon...	227	C11H17NO2S	023705-38-6	86
3	4-Methyl-N-(2-oxobutyl)benzenesu...	241	C11H15NO3S	1000192-14-5	86
4	Methyl 6-((4-methylphenyl)sulfon...	299	C14H21NO4S	1000504-41-1	72
5	Benzene, 4-(ethylsulfonyl)-1-met...	184	C9H12O2S	007569-34-8	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
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Sample : 02521-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

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

TIC Library : C:\Database\NIST20.L
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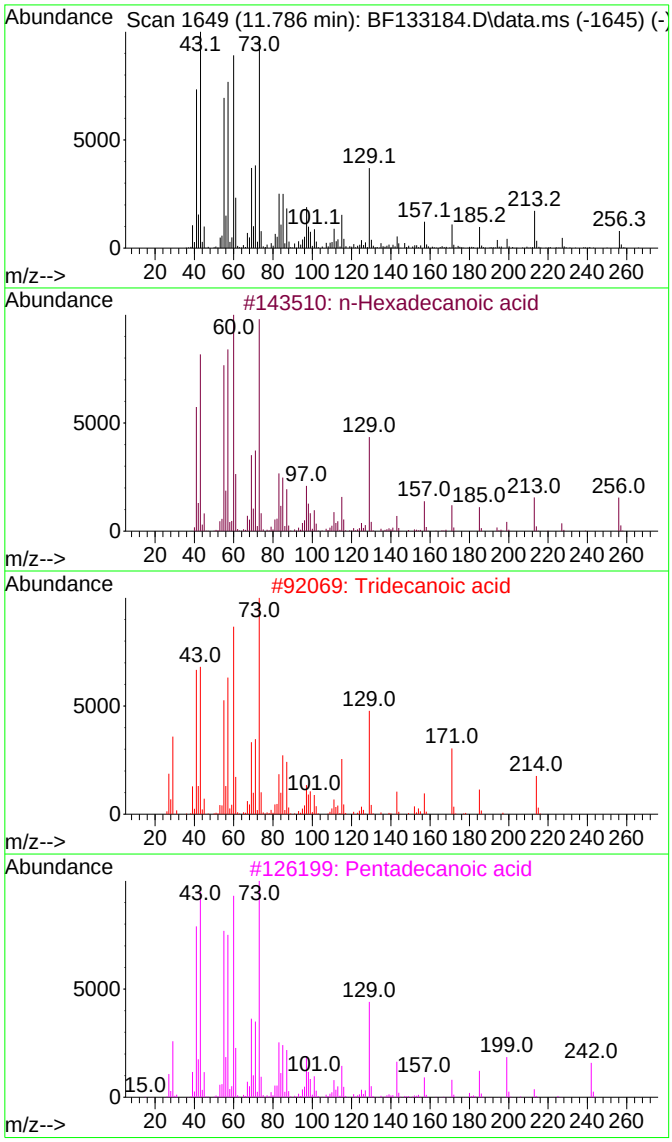
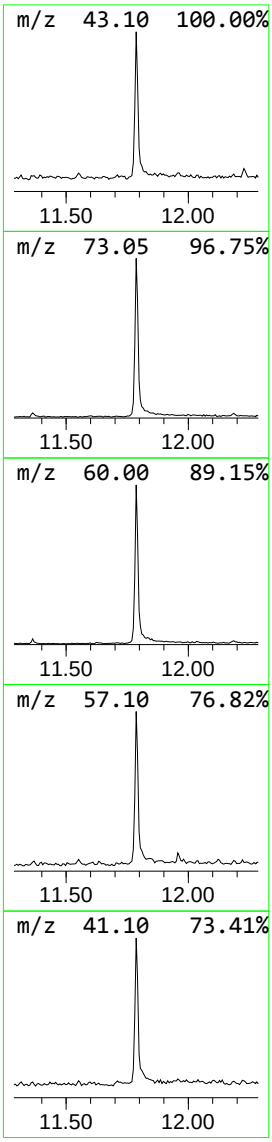
Peak Number 9 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.786	9.85 ng	936569	Phenanthrene-d10	11.245

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	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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Data File : BF133184.D
Acq On : 02 May 2023 12:42
Operator : CG\JU
Sample : 02521-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-15

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

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

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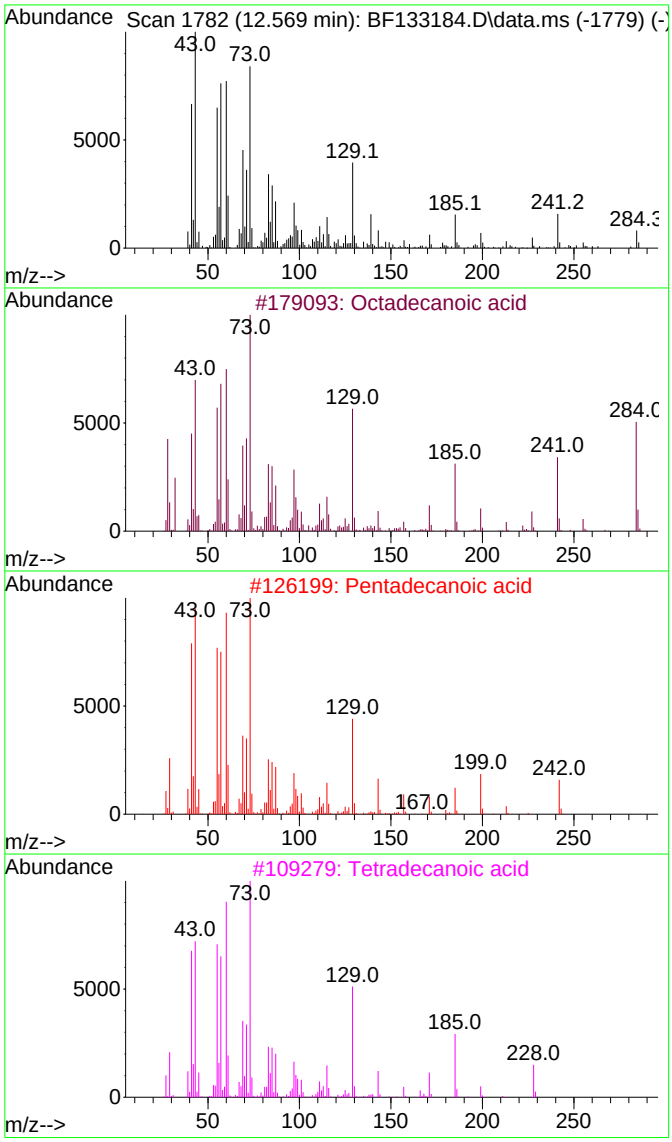
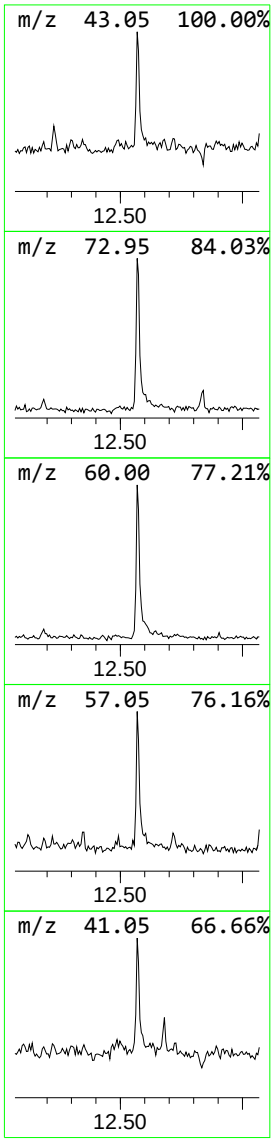
Peak Number 10 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.569	3.77 ng	261514	Chrysene-d12	13.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





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Data File : BF133184.D
Acq On : 02 May 2023 12:42
Operator : CG\JU
Sample : 02521-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-15

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

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

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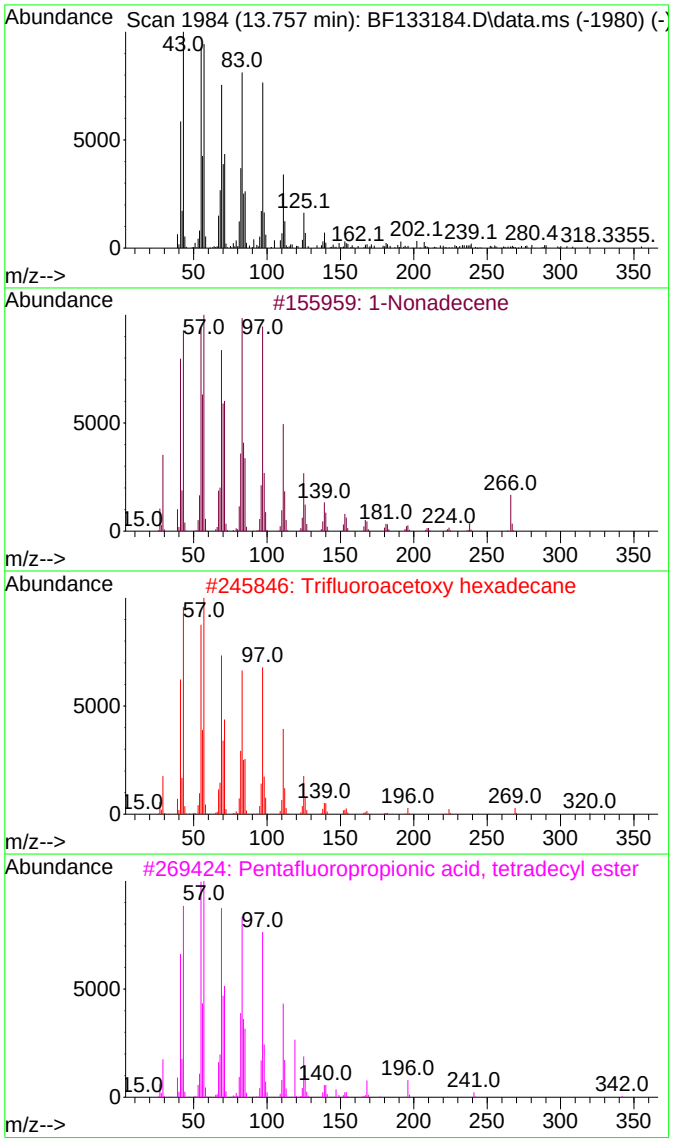
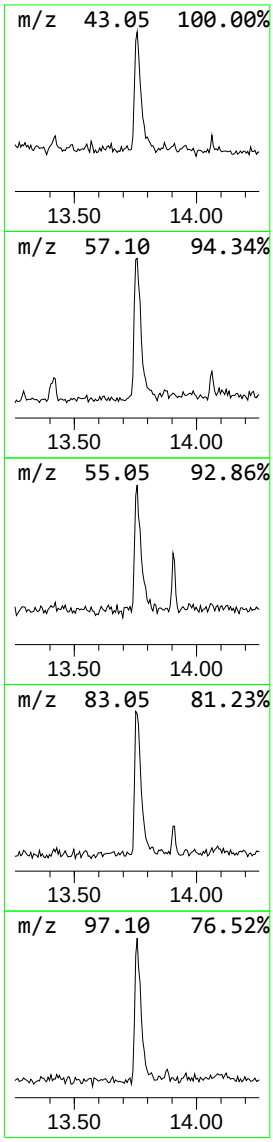
Peak Number 11 1-Nonadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.757	7.15 ng	495410	Chrysene-d12	13.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	99
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
Data File : BF133184.D
Acq On : 02 May 2023 12:42
Operator : CG\JU
Sample : 02521-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-15

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

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

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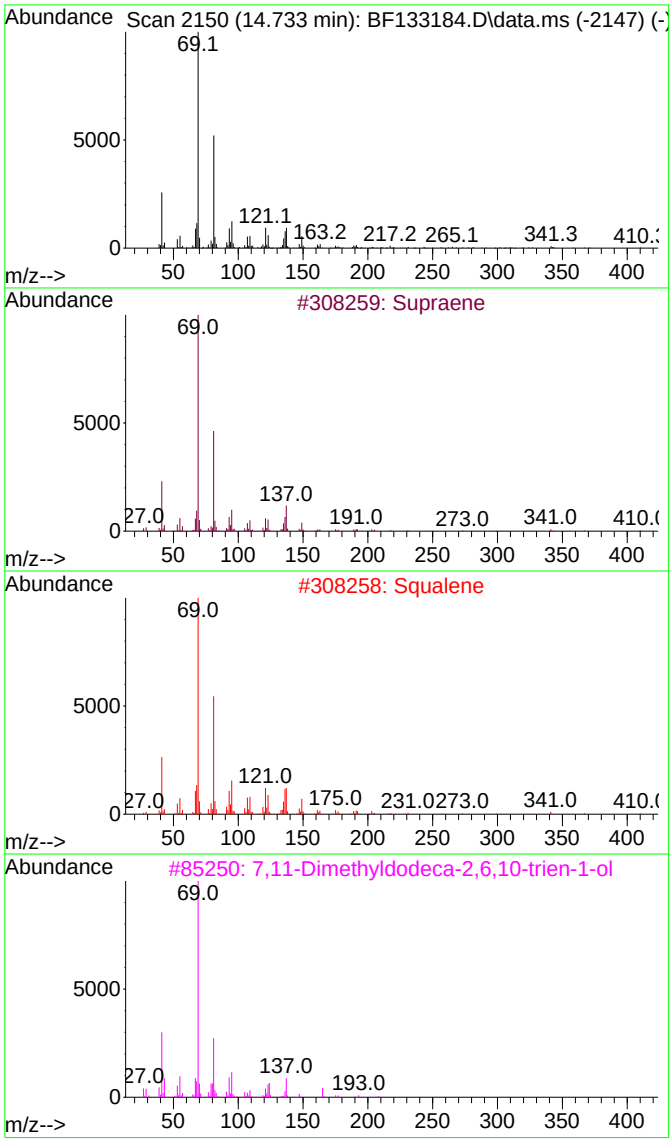
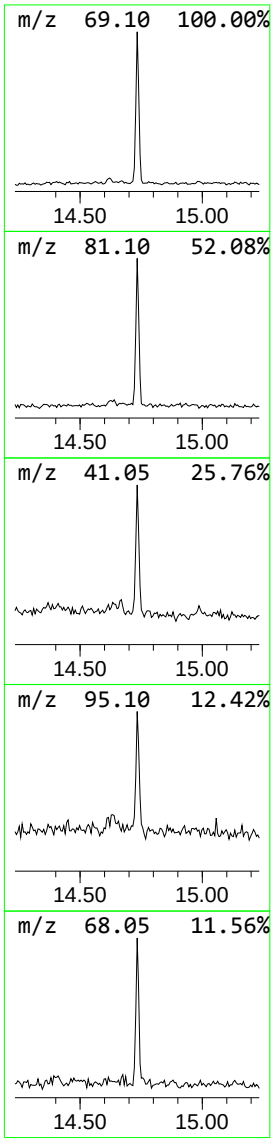
Peak Number 12 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.733	5.01 ng	253530	Perylene-d12	15.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	90
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4	3,7-Dimethyl-1-phenylsulfonyl-2,...	278	C16H22O2S	1000432-27-5	53
5	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
Data File : BF133184.D
Acq On : 02 May 2023 12:42
Operator : CG\JU
Sample : 02521-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-15

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

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Benzene, 1,1'-(...	6.910	2.7	ng	169806	1	6.728	1253210	20.0
Ethanone, 1-(1,...	7.451	7.0	ng	574497	2	8.010	1640140	20.0
Benzene, 1,2,3,...	7.757	2.3	ng	186352	2	8.010	1640140	20.0
Phenol, p-tert-...	8.587	2.7	ng	224706	2	8.010	1640140	20.0
Benzophenone	10.481	3.9	ng	364691	3	9.763	1870990	20.0
2(3H)-Benzothia...	10.657	2.7	ng	256718	4	11.245	1901770	20.0
Benzenesulfonam...	10.839	3.0	ng	287335	4	11.245	1901770	20.0
n-Hexadecanoic ...	11.786	9.8	ng	936569	4	11.245	1901770	20.0
Octadecanoic acid	12.569	3.8	ng	261514	5	13.880	1386070	20.0
1-Nonadecene	13.757	7.2	ng	495410	5	13.880	1386070	20.0
Supraene	14.733	5.0	ng	253530	6	15.304	1011380	20.0