LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102823\
Data File : BF136016.D
Acq On : 28 Oct 2023 20:46
Operator : CG\JU
Sample : 05092-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHRT-20058

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-BF102523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136016.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.051	500	504	510	rVB	78583	88760	3.28%	0.341%
2	5.451	567	572	575	rBV	3009090	2706968	100.00%	10.407%
3	6.451	737	742	745	rBV	2804627	2655614	98.10%	10.210%
4	6.651	773	776	785	rBV	66422	76338	2.82%	0.293%
5	6.822	800	805	809	rBV	1429639	1220099	45.07%	4.691%
6	7.387	896	901	903	rBV	1815384	1693762	62.57%	6.512%
7	8.104	1018	1023	1026	rBV	1987703	1526850	56.40%	5.870%
8	8.345	1060	1064	1066	rBV2	44788	62139	2.30%	0.239%
9	8.398	1070	1073	1076	rVB3	56075	56039	2.07%	0.215%
10	8.569	1100	1102	1105	rVB	71985	60697	2.24%	0.233%
11	8.698	1120	1124	1126	rBV4	42727	53681	1.98%	0.206%
12	8.798	1137	1141	1147	rVB7	52399	77133	2.85%	0.297%
13	8.881	1152	1155	1158	rBV5	47280	54413	2.01%	0.209%
14	8.928	1158	1163	1165	rBV3	128393	162894	6.02%	0.626%
15	8.986	1171	1173	1176	rVB4	66273	67649	2.50%	0.260%
16	9.104	1190	1193	1194	rBV3	58292	56789	2.10%	0.218%
17	9.181	1203	1206	1209	rBV	2611225	2086746	77.09%	8.023%
18	9.222	1210	1213	1215	rBV4	97063	90391	3.34%	0.348%
19	9.263	1216	1220	1225	rBV6	232816	376908	13.92%	1.449%
20	9.304	1225	1227	1229	rBV3	98696	96409	3.56%	0.371%
21	9.334	1230	1232	1234	rVB	107186	74409	2.75%	0.286%
22	9.463	1251	1254	1256	rBV4	79746	89670	3.31%	0.345%
23	9.498	1257	1260	1262	rBV2	217678	238077	8.79%	0.915%
24	9.534	1263	1266	1270	rVB	793197	746114	27.56%	2.869%
25	9.569	1270	1272	1274	rBV2	220856	218891	8.09%	0.842%
26	9.681	1289	1291	1293	rBV3	147023	102098	3.77%	0.393%
27	9.733	1297	1300	1302	rBV3	280577	357708	13.21%	1.375%
28	9.775	1304	1307	1310	rVB4	586411	578943	21.39%	2.226%
29	9.810	1310	1313	1316	rBV5	212716	338414	12.50%	1.301%
30	9.863	1316	1322	1326	rBV	2169583	2410564	89.05%	9.268%
31	10.275	1389	1392	1395	rBV2	760279	755188	27.90%	2.903%
32	10.657	1454	1457	1459	rBV	1480838	1350562	49.89%	5.192%
33	11.363	1575	1577	1579	rVB	1081420	779653	28.80%	2.998%
34	12.957	1845	1848	1853	rVB	1747756	1631733	60.28%	6.273%
35	14.010	2023	2027	2030	rVB	1171770	1028311	37.99%	3.954%
36	14.521	2111	2114	2120	rVB	154773	174284	6.44%	0.670%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102823\
Data File : BF136016.D
Acq On : 28 Oct 2023 20:46
Operator : CG\JU
Sample : 05092-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-20058

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-BF102523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.792	2156	2160	2170	rBV	279095	371049	13.71%	1.427%
38	14.892	2174	2177	2182	rVB	75109	74697	2.76%	0.287%
39	15.168	2221	2224	2230	rVB	63270	70168	2.59%	0.270%
40	15.492	2274	2279	2285	rBV	866956	1125119	41.56%	4.326%
41	15.774	2323	2327	2332	rBV2	55924	82124	3.03%	0.316%
42	16.874	2508	2514	2522	rVB2	70355	142039	5.25%	0.546%

Sum of corrected areas: 26010094

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102823\
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Instrument :
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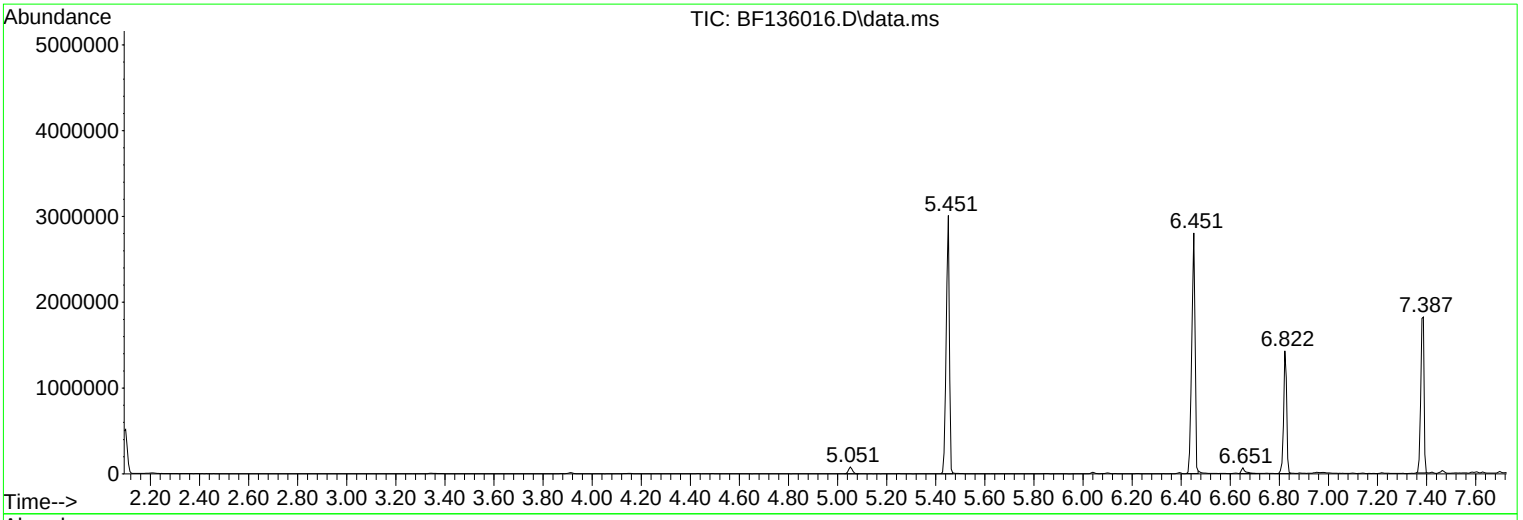
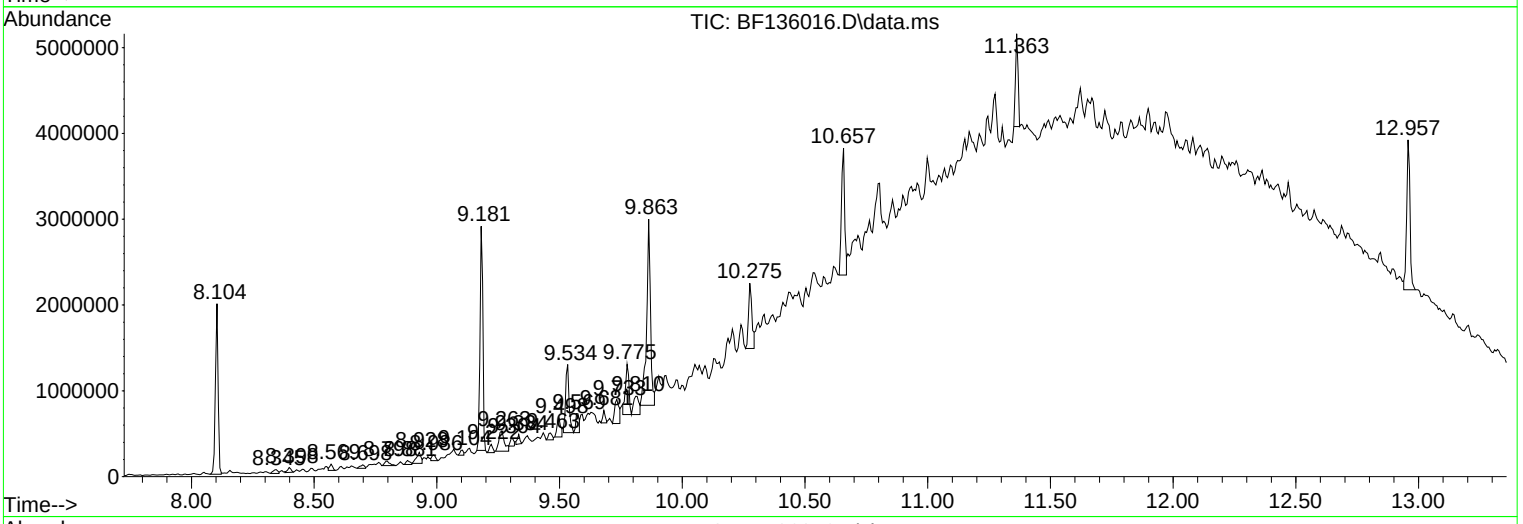
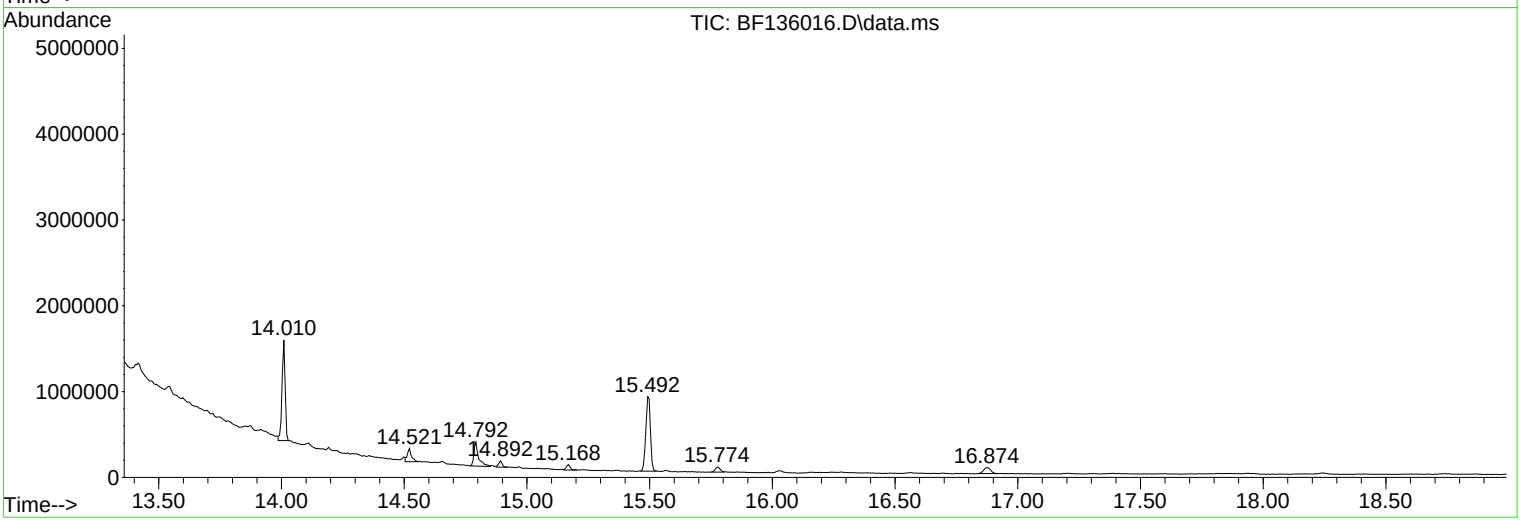
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Data File : BF136016.D
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Operator : CG\JU
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Instrument :
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ClientSampleId :
CHRT-20058

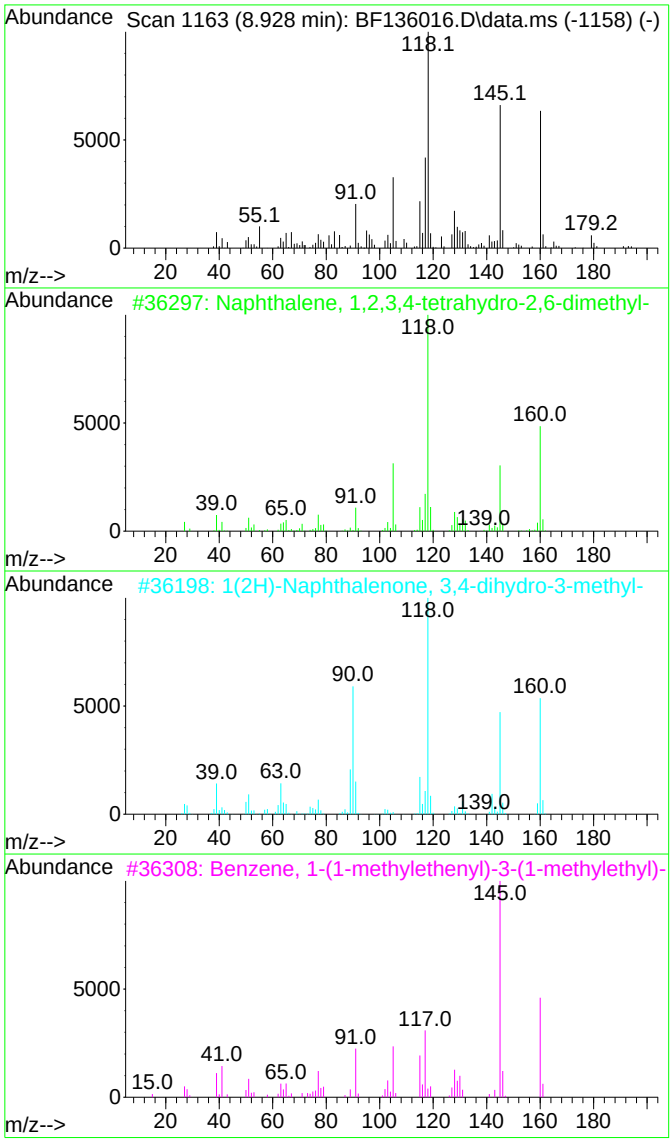
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

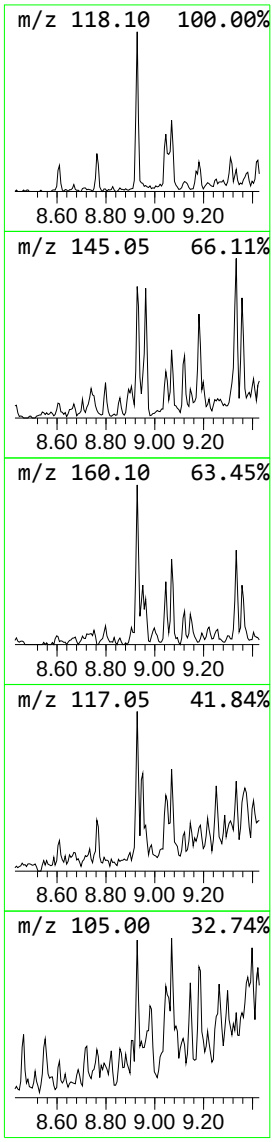
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.928	2.13 ng	162894	Naphthalene-d8	8.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	76
2	1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	014944-23-1	68
3	Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	55
4	2,4-Dimethylphenylacetonitrile	145	C10H11N	068429-53-8	52
5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102823\
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Sample : 05092-01
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-20058

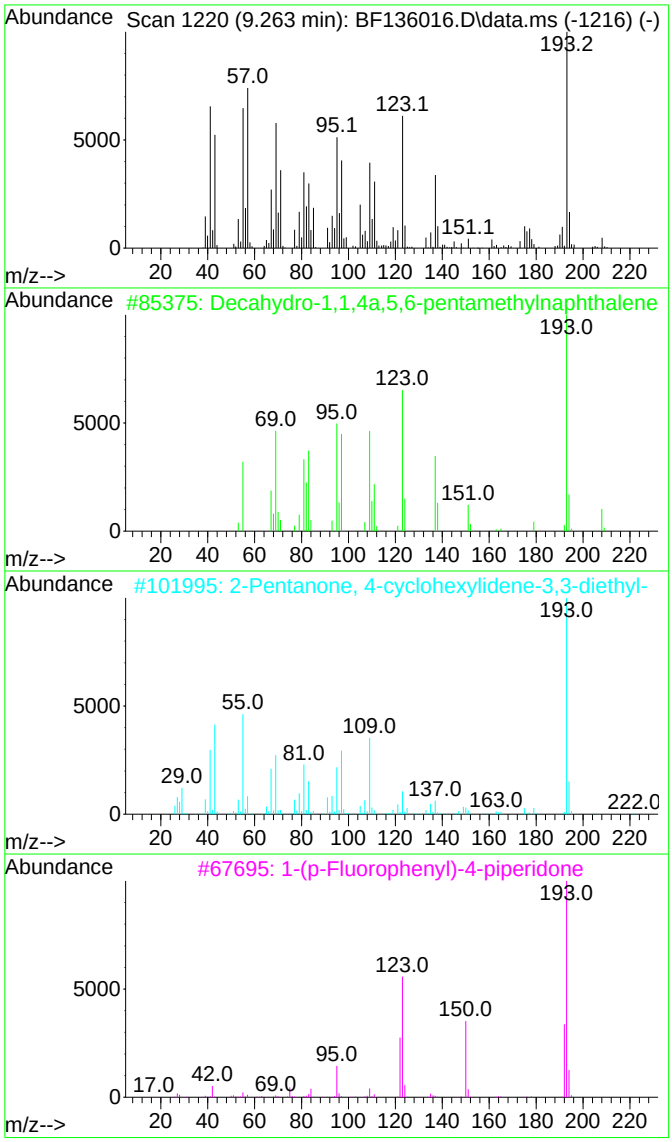
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

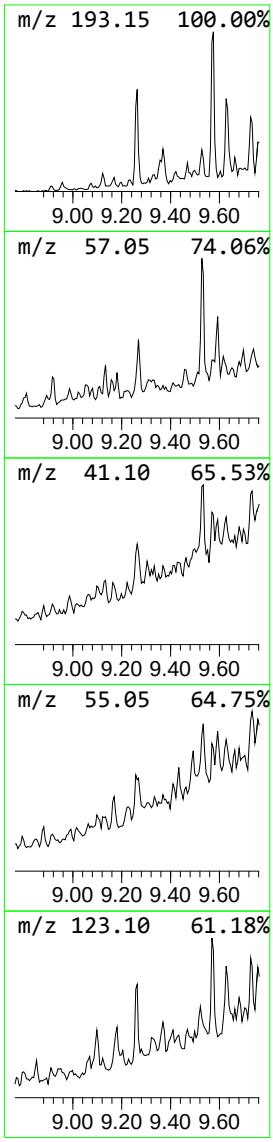
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.263	3.13 ng	376908	Acenaphthene-d10	9.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	78
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	52
3	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38
4	Acridine, 9-methyl-	193	C14H11N	000611-64-3	38
5	Vinyltris(cyclopropyl)silane	178	C11H18Si	1000109-97-3	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102823\
Data File : BF136016.D
Acq On : 28 Oct 2023 20:46
Operator : CG\JU
Sample : 05092-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-20058

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

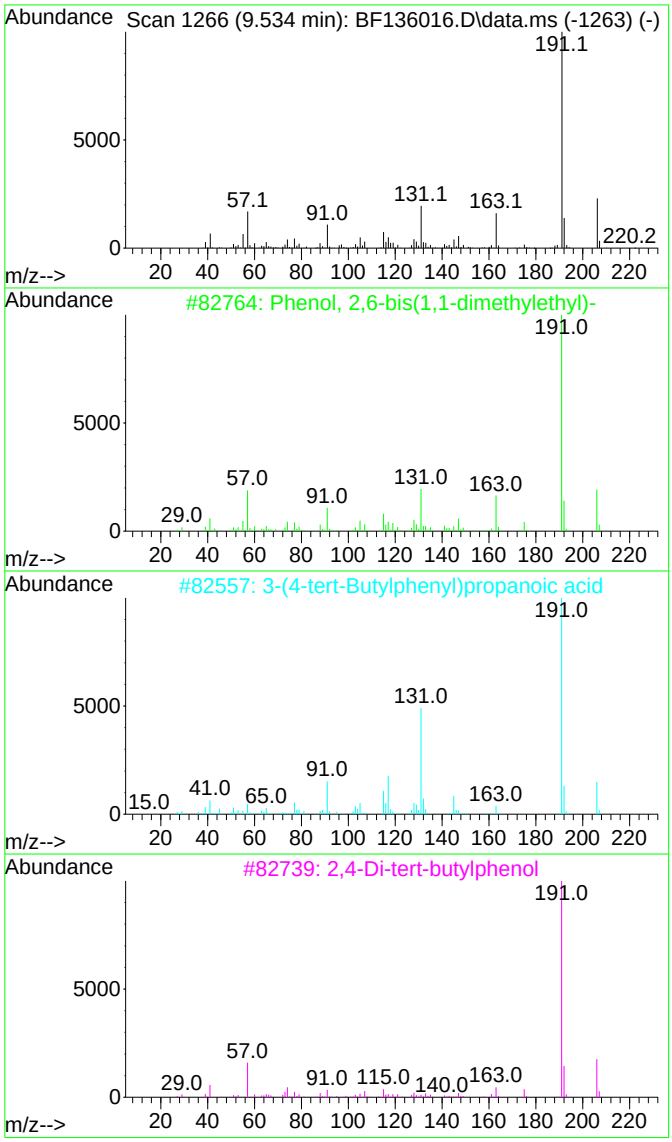
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

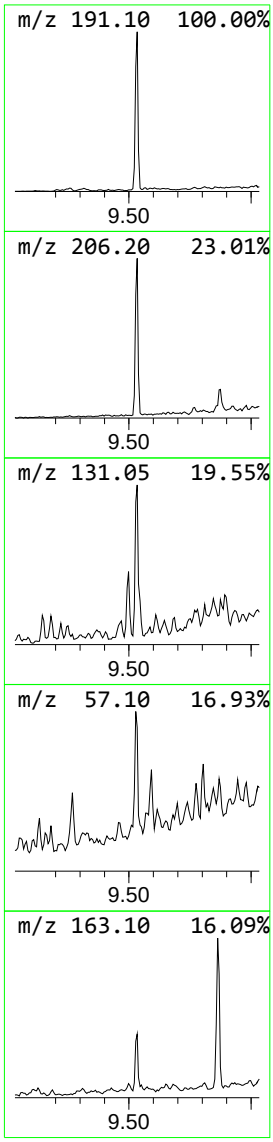
****

Peak Number 3 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.534	6.19 ng	746114	Acenaphthene-d10	9.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	94
2	3-(4-tert-Butylphenyl)propanoic ...	206	C13H18O2	001208-64-6	87
3	2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	76
4	Oxirane, [[4-(1,1-dimethylethyl)...	206	C13H18O2	003101-60-8	70
5	Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102823\
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Operator : CG\JU
Sample : 05092-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-20058

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

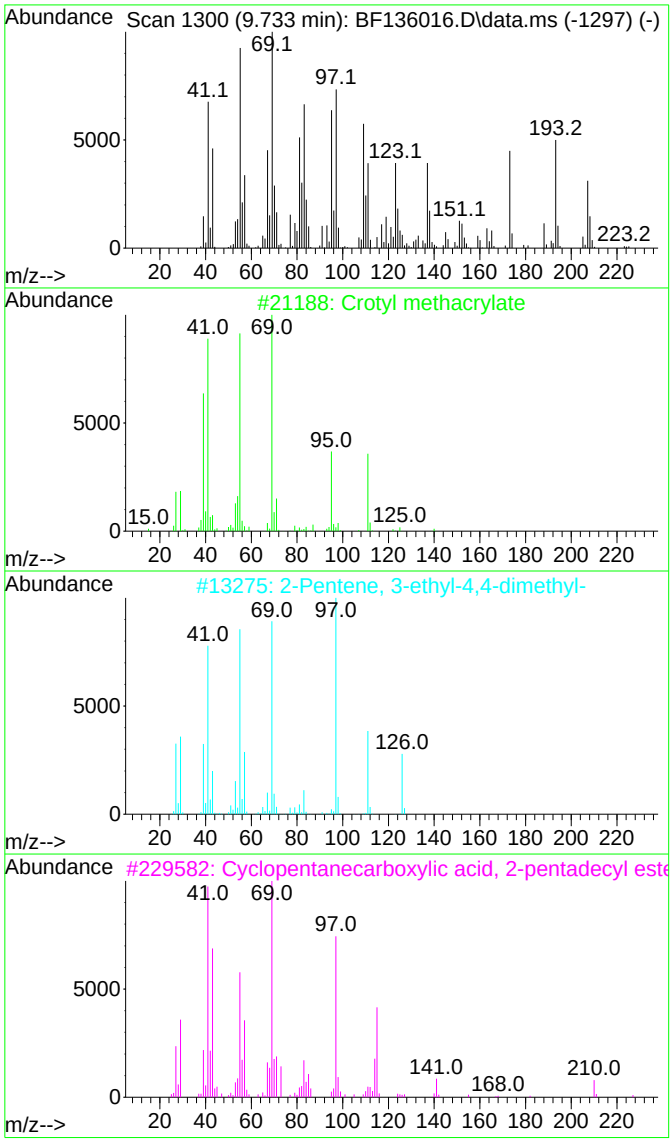
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

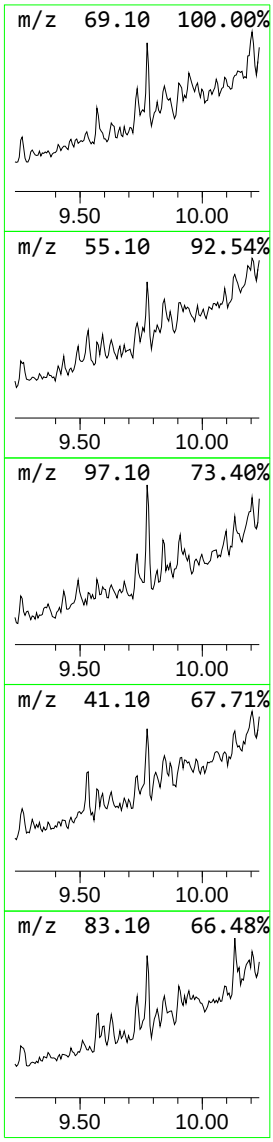
****

Peak Number 4 unknown9.733 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.733	2.97 ng	357708	Acenaphthene-d10	9.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Crotyl methacrylate	140	C8H12O2	007376-45-6	35
2	2-Pentene, 3-ethyl-4,4-dimethyl-	126	C9H18	053907-59-8	22
3	Cyclopentanecarboxylic acid, 2-p...	324	C21H40O2	1010280-59-0	22
4	(2,4-Dimethylcyclohexyl)methanol...	142	C9H18O	1000499-02-8	22
5	1-Decene, 10-bromo-	218	C10H19Br	062871-09-4	22





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Data File : BF136016.D
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Sample : 05092-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-20058

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

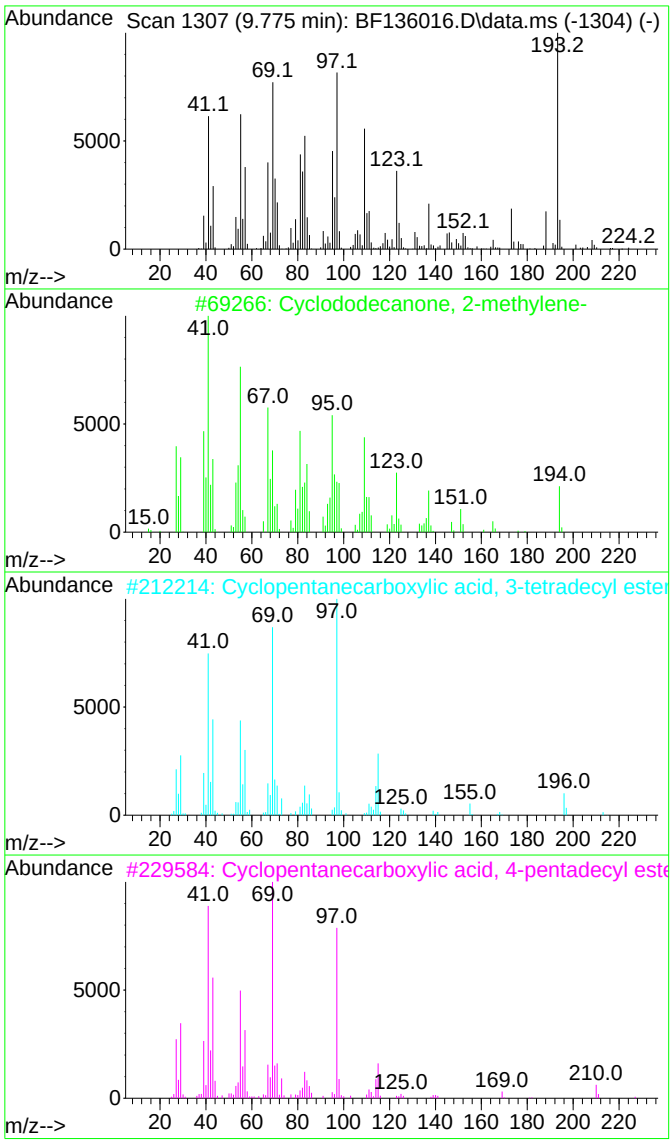
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

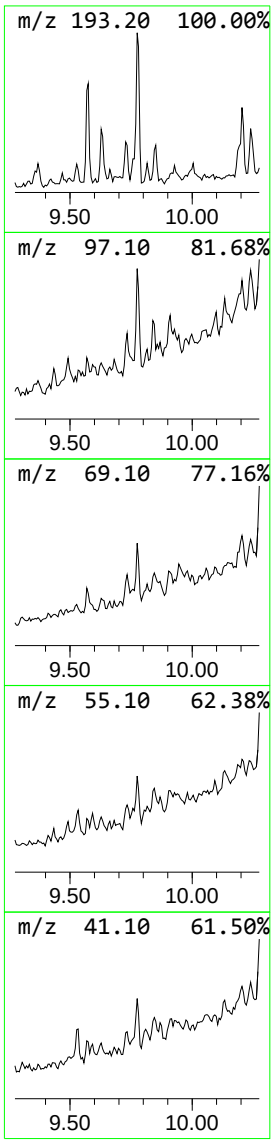
****

Peak Number 5 unknown9.775 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.775	4.80 ng	578943	Acenaphthene-d10	9.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	30
2	Cyclopentanecarboxylic acid, 3-t...	310	C20H38O2	1000280-58-8	27
3	Cyclopentanecarboxylic acid, 4-p...	324	C21H40O2	1000280-59-2	27
4	Cyclopentanecarboxylic acid, 3-t...	296	C19H36O2	1000280-58-5	27
5	Succinic acid, tridec-2-yn-1-yl ...	420	C26H44O4	1010391-10-5	22





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Misc :
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Instrument :
BNA_F
ClientSampleId :
CHRT-20058

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

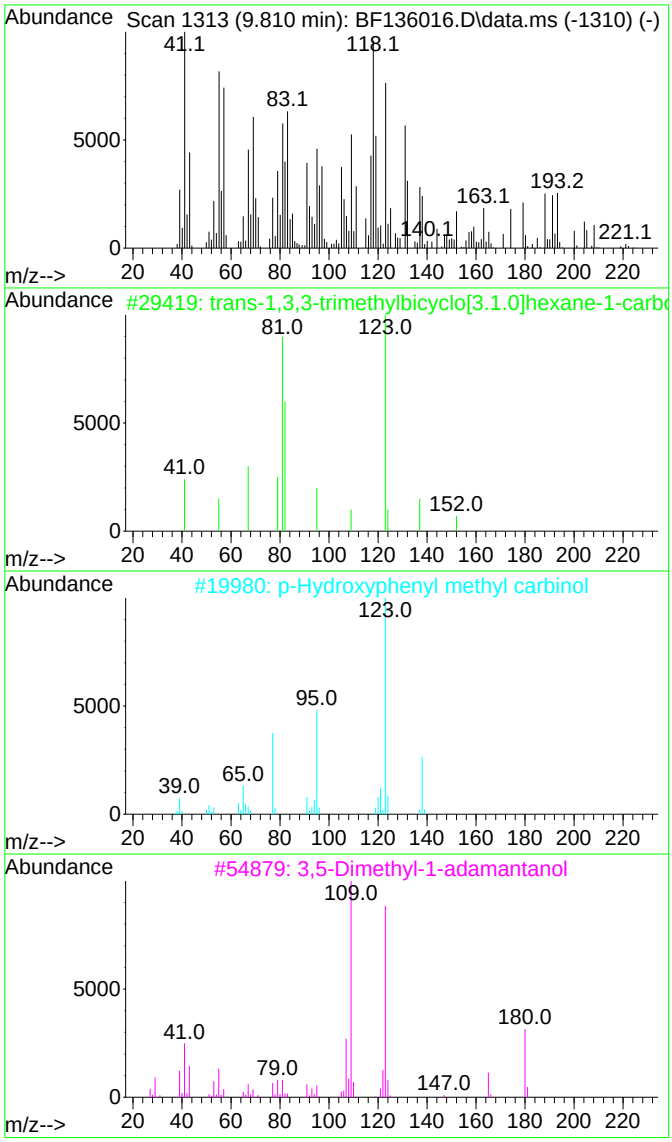
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

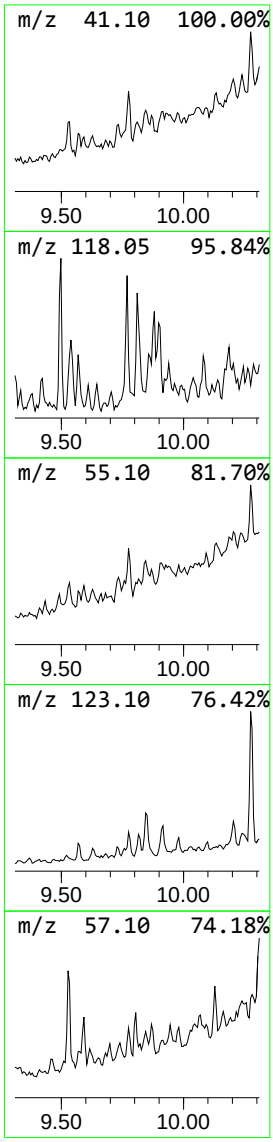
****

Peak Number 6 unknown9.810 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.810	2.81 ng	338414	Acenaphthene-d10	9.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-1,3,3-trimethylbicyclo[3.1...	152	C10H16O	1000365-94-1	25
2	p-Hydroxyphenyl methyl carbinol	138	C8H10O2	002380-91-8	25
3	3,5-Dimethyl-1-adamantanol	180	C12H20O	000707-37-9	20
4	Cyclopentane, 1-methyl-1-(2-meth...	138	C10H18	074764-47-9	20
5	Cyclopentene, 1,3-dimethyl-2-(1-...	138	C10H18	061142-32-3	18





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

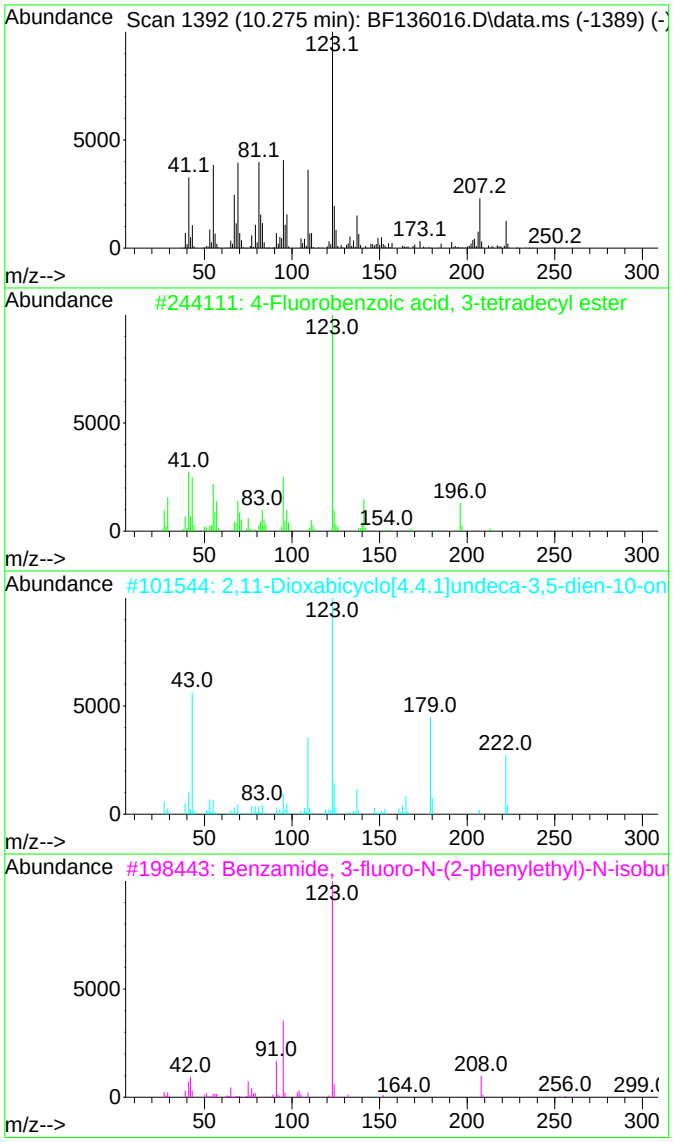
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

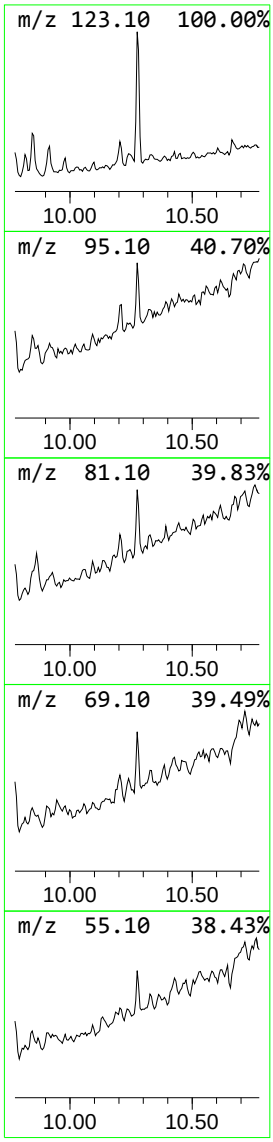
****

Peak Number 7 4-Fluorobenzoic acid, 3-tet... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.275	6.27 ng	755188	Acenaphthene-d10	9.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Fluorobenzoic acid, 3-tetradec...	336	C21H33FO2	1010280-68-1	50
2	2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	47
3	Benzamide, 3-fluoro-N-(2-phenyle...	299	C19H22FNO	1000451-30-2	43
4	trans-2-(1-Hydroxycyclohexyl)-furan	166	C10H14O2	115754-87-5	43
5	N-[(4-Fluorophenyl)carbonyl]glycine	197	C9H8FNO3	000366-79-0	43





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Data File : BF136016.D
Acq On : 28 Oct 2023 20:46
Operator : CG\JU
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Instrument :
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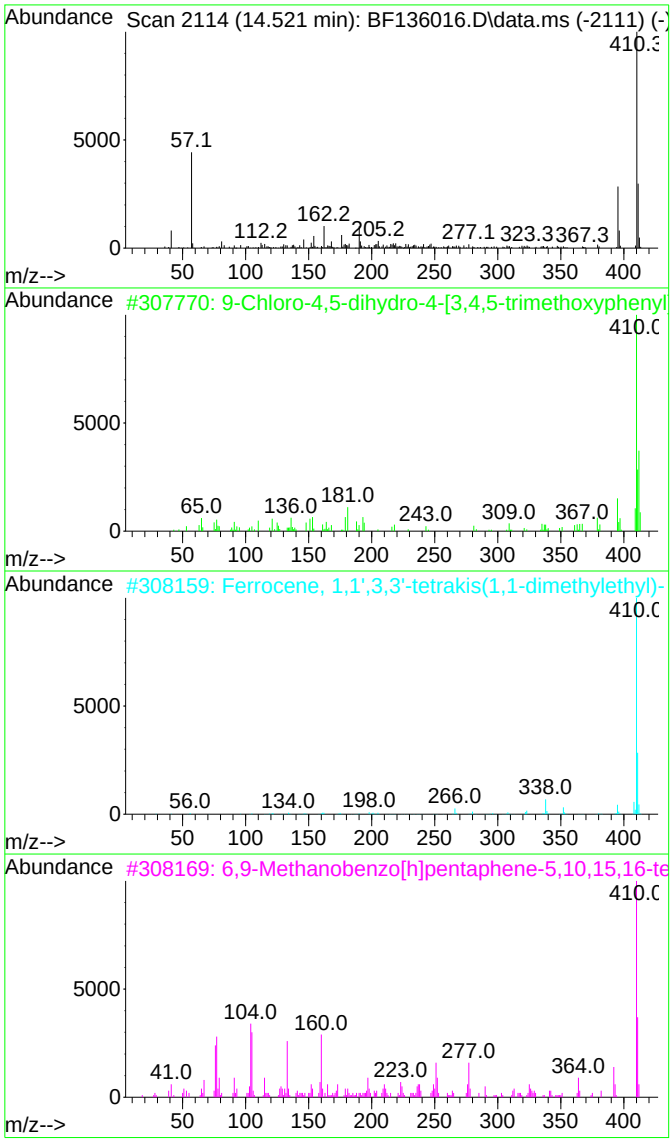
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

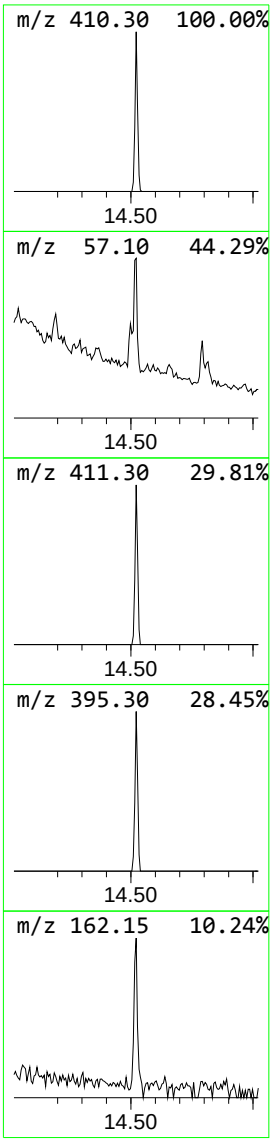
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 9-Chloro-4,5-dihydro-4-[3,4... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.521	3.39 ng	174284	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Chloro-4,5-dihydro-4-[3,4,5-tr...	410	C22H19ClN2O4	1000212-48-1	53
2	Ferrocene, 1,1',3,3'-tetrakis(1,...	410	C26H42Fe	001317-17-5	53
3	6,9-Methanobenzo[h]pentaphene-5,...	410	C27H22O4	057427-50-6	40
4	.DELTA.9-thc tfa	410	C23H29F3O3	086702-79-6	40
5	Acetic acid, (4-chloro-2-methylp...	410	C24H39ClO3	1000415-16-8	28





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Data File : BF136016.D
Acq On : 28 Oct 2023 20:46
Operator : CG\JU
Sample : 05092-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-20058

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

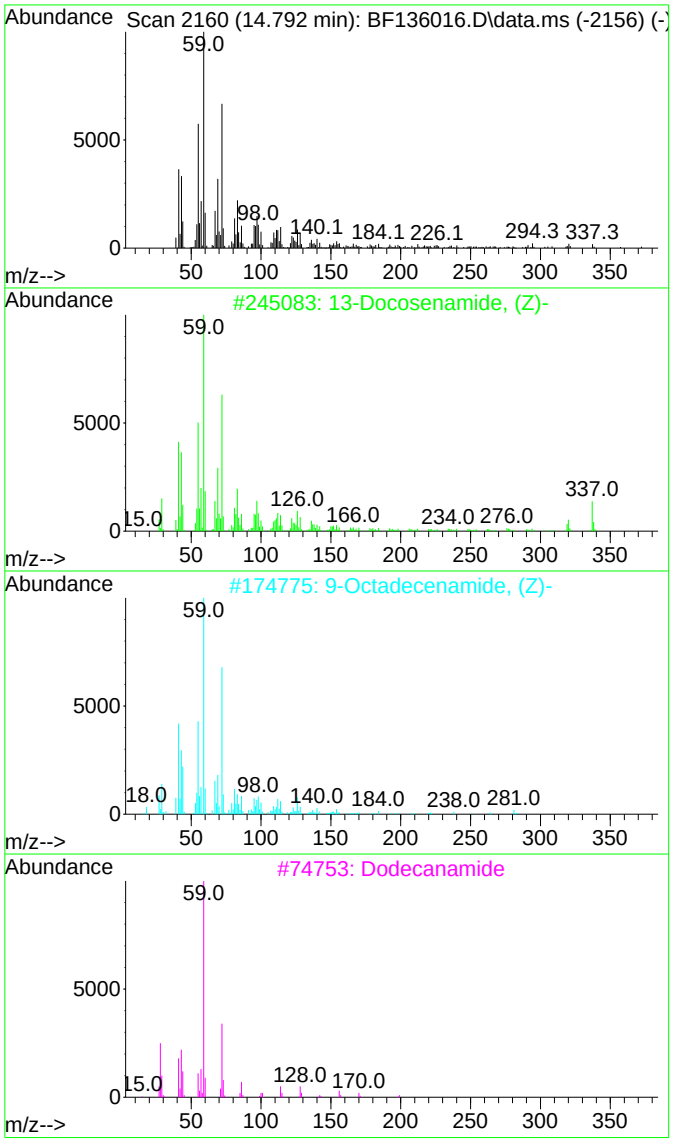
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

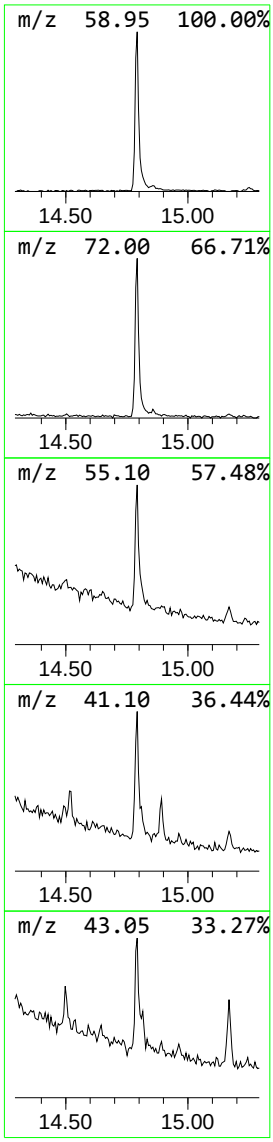
****

Peak Number 9 13-Docosenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.792	6.60 ng	371049	Perylene-d12	15.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
3	Dodecanamide	199	C12H25NO	001120-16-7	60
4	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50
5	4,8,12,16-tetraoxaeicosan-1-ol	306	C16H34O5	1010397-63-6	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102823\
Data File : BF136016.D
Acq On : 28 Oct 2023 20:46
Operator : CG\JU
Sample : 05092-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-20058

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.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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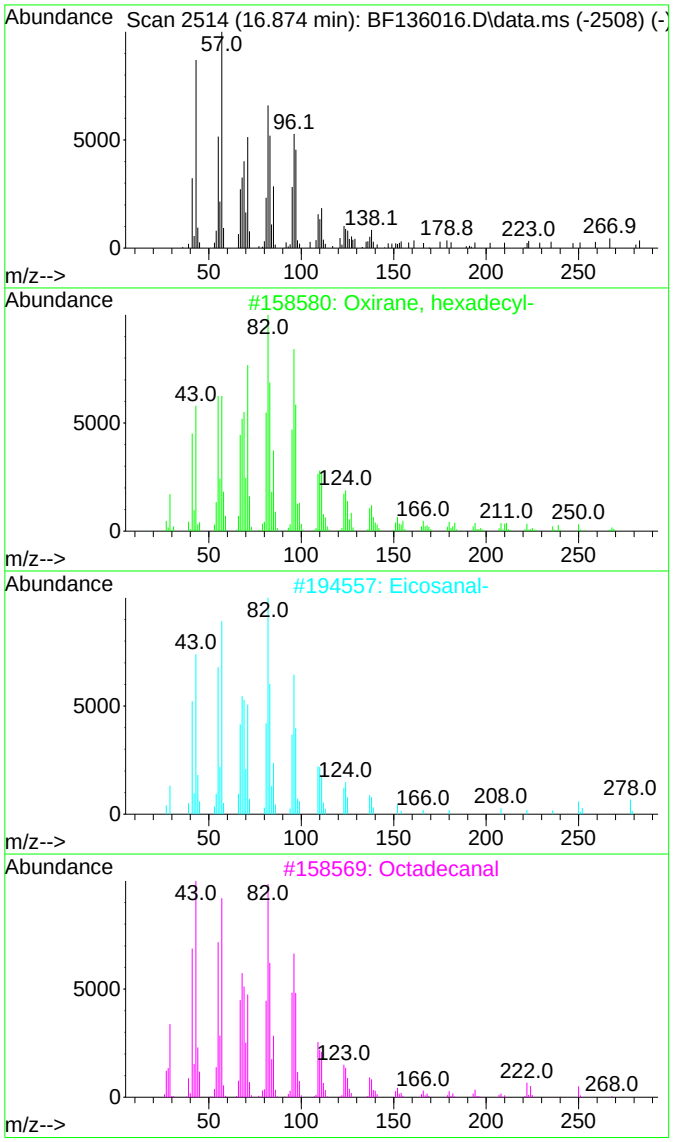
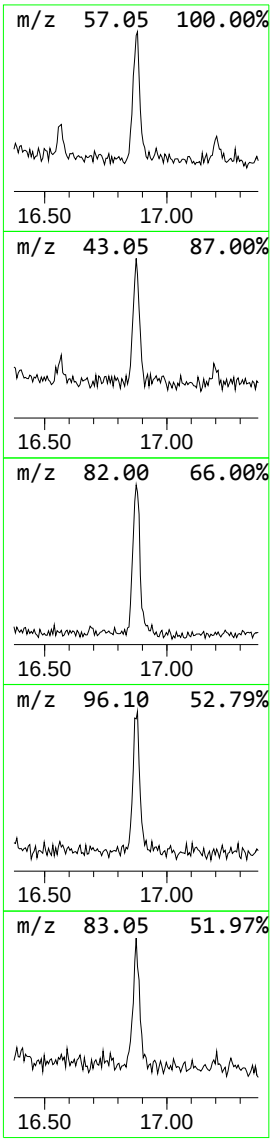
Peak Number 10 Oxirane, hexadecyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.874	2.52 ng	142039	Perylene-d12	15.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	76
2	Eicosanal-	296	C20H40O	002400-66-0	74
3	Octadecanal	268	C18H36O	000638-66-4	68
4	1,19-Eicosadiene	278	C20H38	014811-95-1	62
5	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102823\
Data File : BF136016.D
Acq On : 28 Oct 2023 20:46
Operator : CG\JU
Sample : 05092-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-20058

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.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
Naphthalene, 1,...	8.928	2.1	ng	162894	2	8.104	1526850	20.0
Decahydro-1,1,4...	9.263	3.1	ng	376908	3	9.863	2410560	20.0
Phenol, 2,6-bis...	9.534	6.2	ng	746114	3	9.863	2410560	20.0
unknown9.733	9.733	3.0	ng	357708	3	9.863	2410560	20.0
unknown9.775	9.775	4.8	ng	578943	3	9.863	2410560	20.0
unknown9.810	9.810	2.8	ng	338414	3	9.863	2410560	20.0
4-Fluorobenzoic...	10.275	6.3	ng	755188	3	9.863	2410560	20.0
9-Chloro-4,5-di...	14.521	3.4	ng	174284	5	14.010	1028310	20.0
13-Docosenamide...	14.792	6.6	ng	371049	6	15.492	1125120	20.0
Oxirane, hexade...	16.874	2.5	ng	142039	6	15.492	1125120	20.0