LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082818\
Data File : BF108559.D
Acq On : 28 Aug 2018 16:58
Operator : JU/SJ
Sample : J4523-02 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-2

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-BF080818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.237	489	493	501	rBV	36022	55768	4.21%	0.319%
2	5.495	534	537	540	rBV	20259	24625	1.86%	0.141%
3	5.601	551	555	559	rBV2	42555	72677	5.48%	0.416%
4	5.642	559	562	587	rVB	499019	1024613	77.29%	5.860%
5	5.854	595	598	601	rBV	22620	23827	1.80%	0.136%
6	5.889	601	604	610	rVB2	34718	48631	3.67%	0.278%
7	6.519	707	711	715	rBV	68335	76372	5.76%	0.437%
8	6.554	715	717	721	rVV	44107	47264	3.57%	0.270%
9	6.595	721	724	728	rVV	50767	44967	3.39%	0.257%
10	6.636	728	731	751	rVV	745522	1315088	99.20%	7.522%
11	6.778	751	755	760	rVV	1070886	1178431	88.89%	6.740%
12	6.819	760	762	768	rVB	182416	168371	12.70%	0.963%
13	7.001	789	793	799	rBV	687956	731952	55.21%	4.186%
14	7.048	799	801	809	rVB2	48837	64479	4.86%	0.369%
15	7.154	815	819	830	rBV	935054	941017	70.98%	5.382%
16	7.266	835	838	842	rVV2	51634	58307	4.40%	0.333%
17	7.307	842	845	852	rVB3	90154	103361	7.80%	0.591%
18	7.478	872	874	878	rVB	28962	24496	1.85%	0.140%
19	7.525	878	882	885	rBV2	82957	90627	6.84%	0.518%
20	7.560	885	888	897	rVB	777923	795405	60.00%	4.549%
21	7.760	919	922	924	rBV	33401	29901	2.26%	0.171%
22	7.783	924	926	934	rVB	47943	47311	3.57%	0.271%
23	7.948	952	954	958	rBV2	31735	29516	2.23%	0.169%
24	8.013	962	965	967	rVV2	73825	78640	5.93%	0.450%
25	8.036	967	969	973	rVB3	38334	37225	2.81%	0.213%
26	8.242	1001	1004	1006	rBV2	20796	24905	1.88%	0.142%
27	8.283	1007	1011	1020	rVB	1028294	1038730	78.35%	5.941%
28	8.554	1054	1057	1062	rVB4	21559	28225	2.13%	0.161%
29	8.995	1129	1132	1138	rVB	109981	98871	7.46%	0.565%
30	9.060	1138	1143	1147	rBV	59549	91520	6.90%	0.523%
31	9.095	1147	1149	1154	rVB	55231	57298	4.32%	0.328%
32	9.354	1189	1193	1198	rBV	1682220	1325753	100.00%	7.583%
33	9.624	1233	1239	1243	rBV2	19729	30100	2.27%	0.172%
34	9.695	1247	1251	1254	rBV3	21426	25168	1.90%	0.144%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082818\
Data File : BF108559.D
Acq On : 28 Aug 2018 16:58
Operator : JU/SJ
Sample : J4523-02 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-2

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-BF080818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.748	1257	1260	1263	rVB	130388	105268	7.94%	0.602%
36	10.042	1304	1310	1318	rBV	1065705	994809	75.04%	5.690%
37	10.224	1336	1341	1347	rVB9	24806	46611	3.52%	0.267%
38	10.366	1359	1365	1368	rBV4	26871	41424	3.12%	0.237%
39	10.448	1373	1379	1382	rBV4	44647	62028	4.68%	0.355%
40	10.666	1413	1416	1420	rBV2	17861	26400	1.99%	0.151%
41	10.836	1441	1445	1452	rBV	822362	743292	56.07%	4.251%
42	10.936	1458	1462	1469	rVB3	41206	67621	5.10%	0.387%
43	11.177	1500	1503	1507	rVB4	42718	44625	3.37%	0.255%
44	11.248	1513	1515	1520	rBV	44754	48938	3.69%	0.280%
45	11.383	1534	1538	1540	rBV2	63617	103832	7.83%	0.594%
46	11.542	1561	1565	1568	rBV	920820	819427	61.81%	4.687%
47	11.566	1568	1569	1572	rVB	50622	29999	2.26%	0.172%
48	11.683	1587	1589	1592	rBV4	37977	43707	3.30%	0.250%
49	11.801	1607	1609	1614	rBV2	38691	54112	4.08%	0.309%
50	12.048	1647	1651	1656	rBV	407444	450938	34.01%	2.579%
51	12.836	1782	1785	1791	rBV	283692	292476	22.06%	1.673%
52	13.124	1831	1834	1838	rVB	1038989	882925	66.60%	5.050%
53	14.148	2005	2008	2013	rBV	538915	452578	34.14%	2.589%
54	14.201	2014	2017	2020	rBV	786251	710449	53.59%	4.063%
55	14.571	2077	2080	2084	rVB2	1151970	1028756	77.60%	5.884%
56	15.771	2281	2284	2288	rVB	473545	600382	45.29%	3.434%

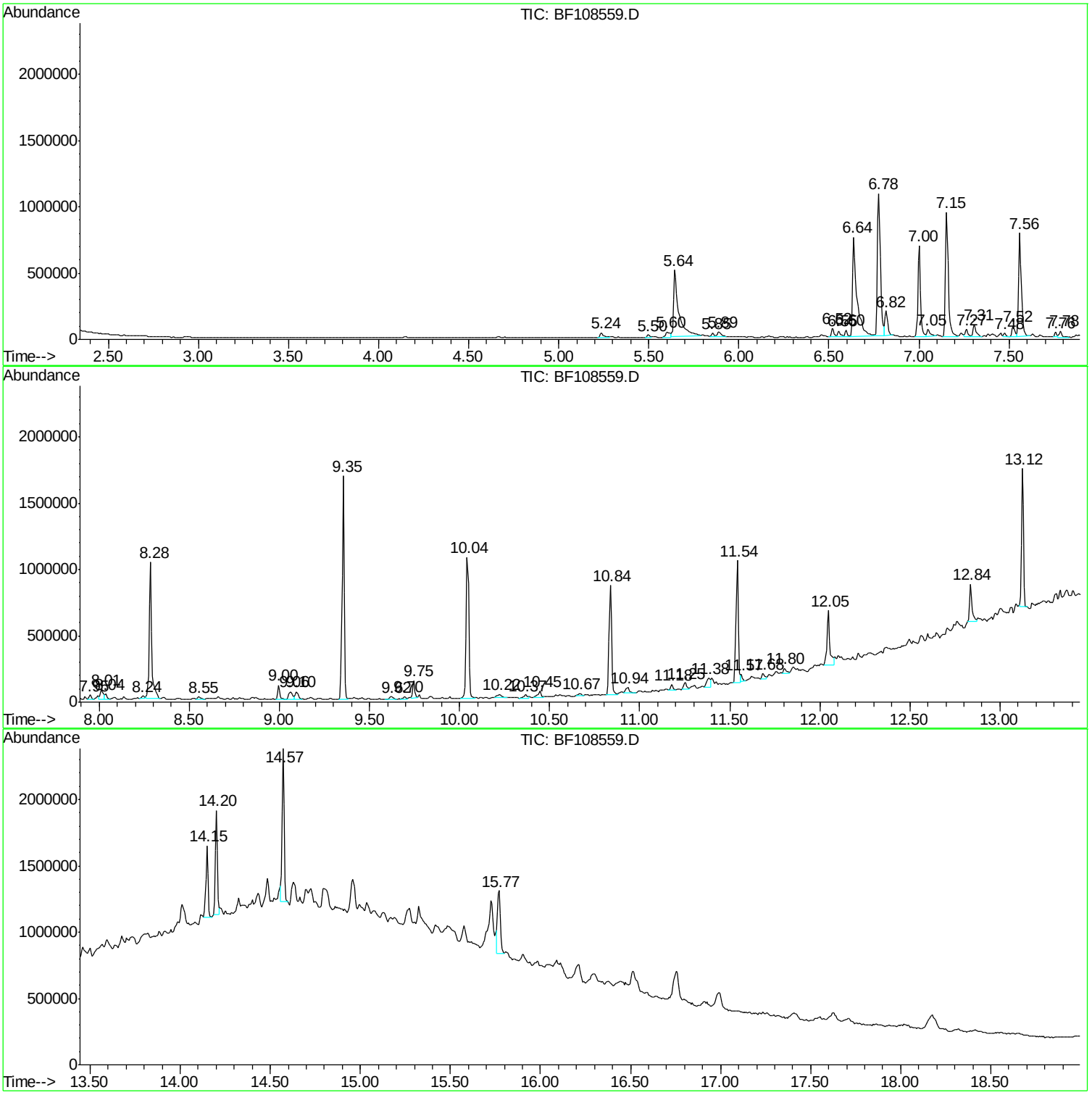
Sum of corrected areas: 17484038

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082818\
Data File : BF108559.D
Acq On : 28 Aug 2018 16:58
Operator : JU/SJ
Sample : J4523-02 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082818\
Data File : BF108559.D
Acq On : 28 Aug 2018 16:58
Operator : JU/SJ
Sample : J4523-02 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

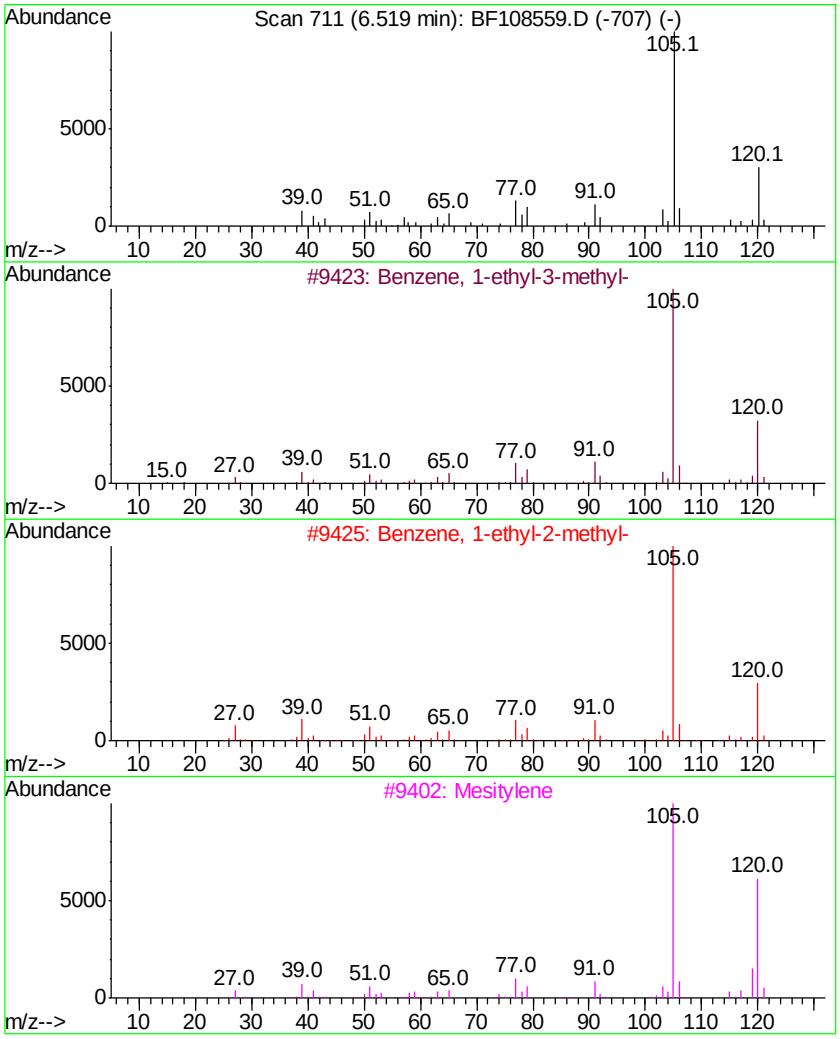
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

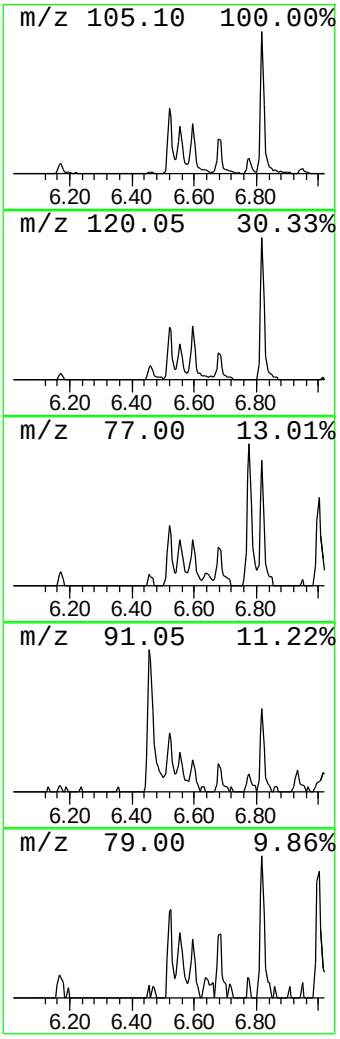
****

Peak Number 1 Benzene, 1-ethyl-3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	2.09 ng	76372	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082818\
Data File : BF108559.D
Acq On : 28 Aug 2018 16:58
Operator : JU/SJ
Sample : J4523-02 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

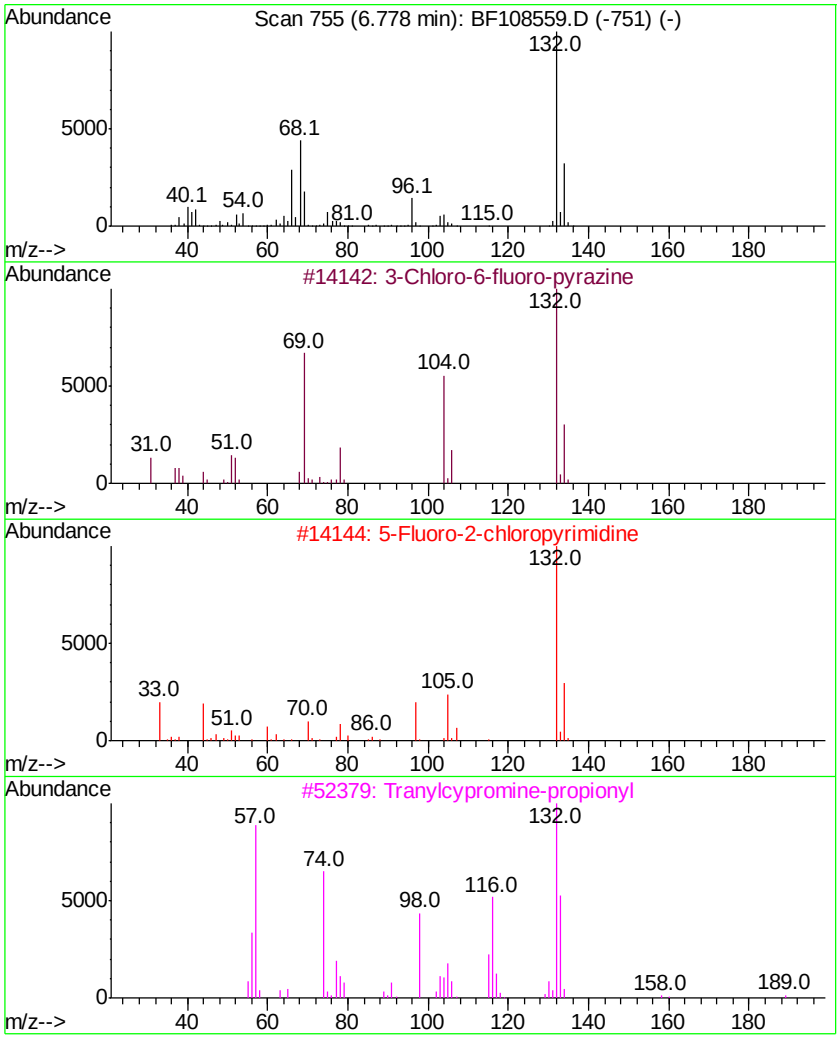
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

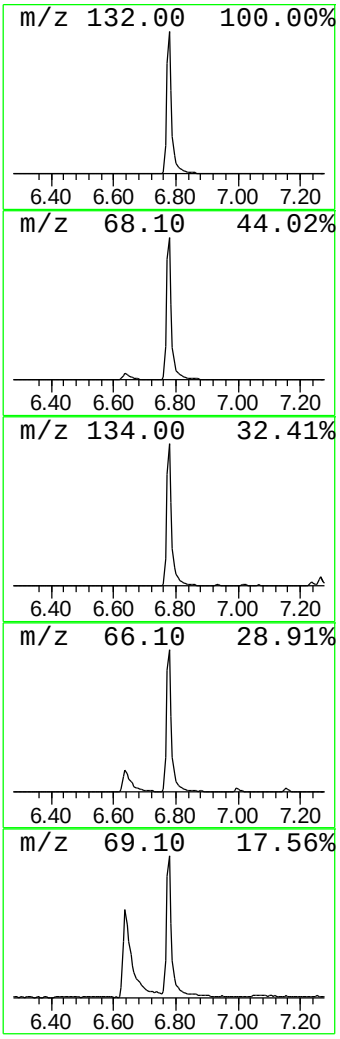
****

Peak Number 2 unknown6.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	32.20 ng	1178430	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082818\
Data File : BF108559.D
Acq On : 28 Aug 2018 16:58
Operator : JU/SJ
Sample : J4523-02 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

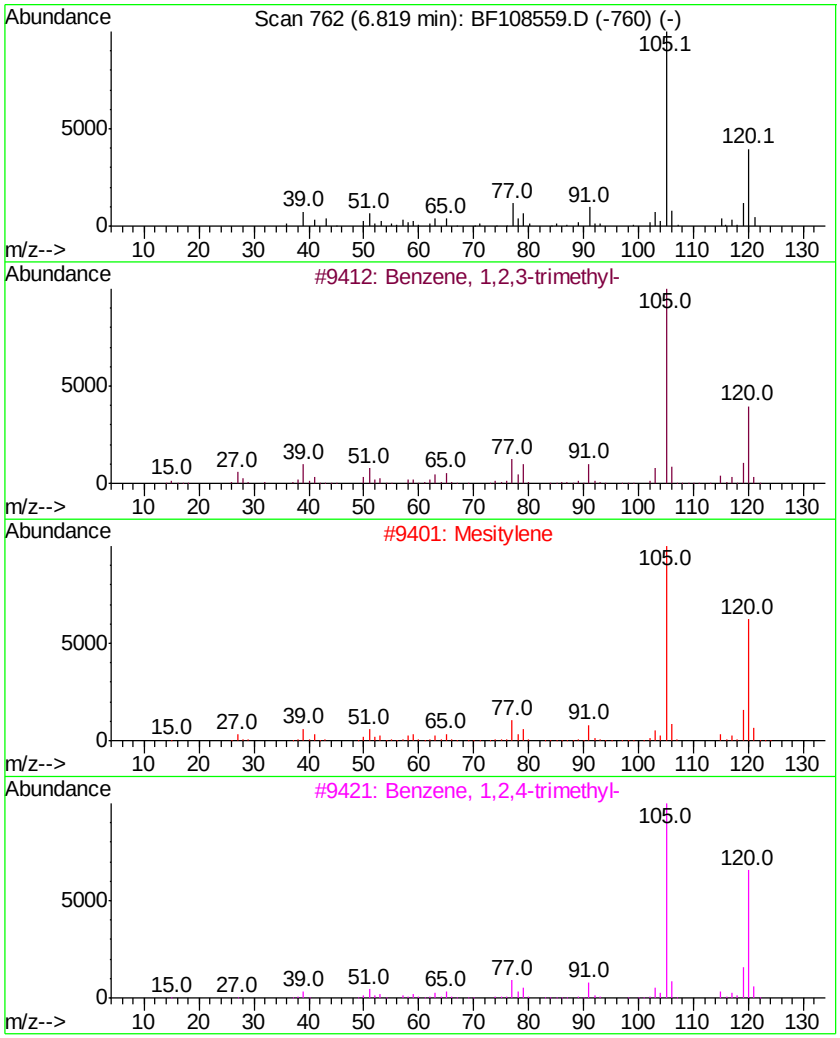
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

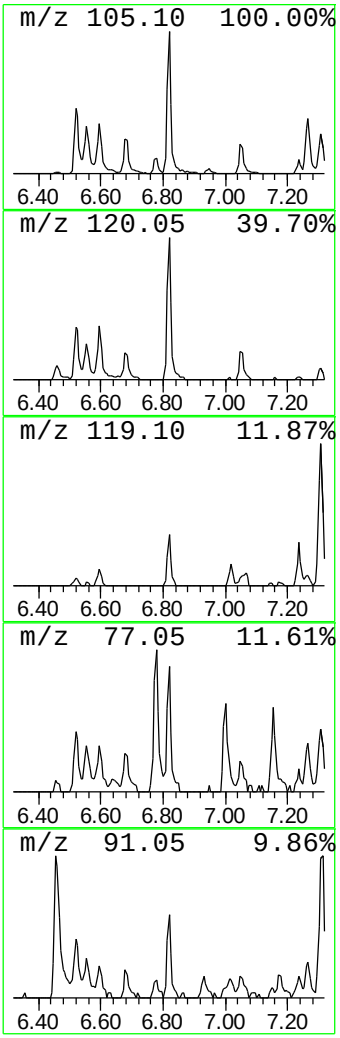
****

Peak Number 3 Benzene, 1,2,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.82	4.60 ng	168371	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2	Mesitylene	120	C9H12	000108-67-8	95
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082818\
Data File : BF108559.D
Acq On : 28 Aug 2018 16:58
Operator : JU/SJ
Sample : J4523-02 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

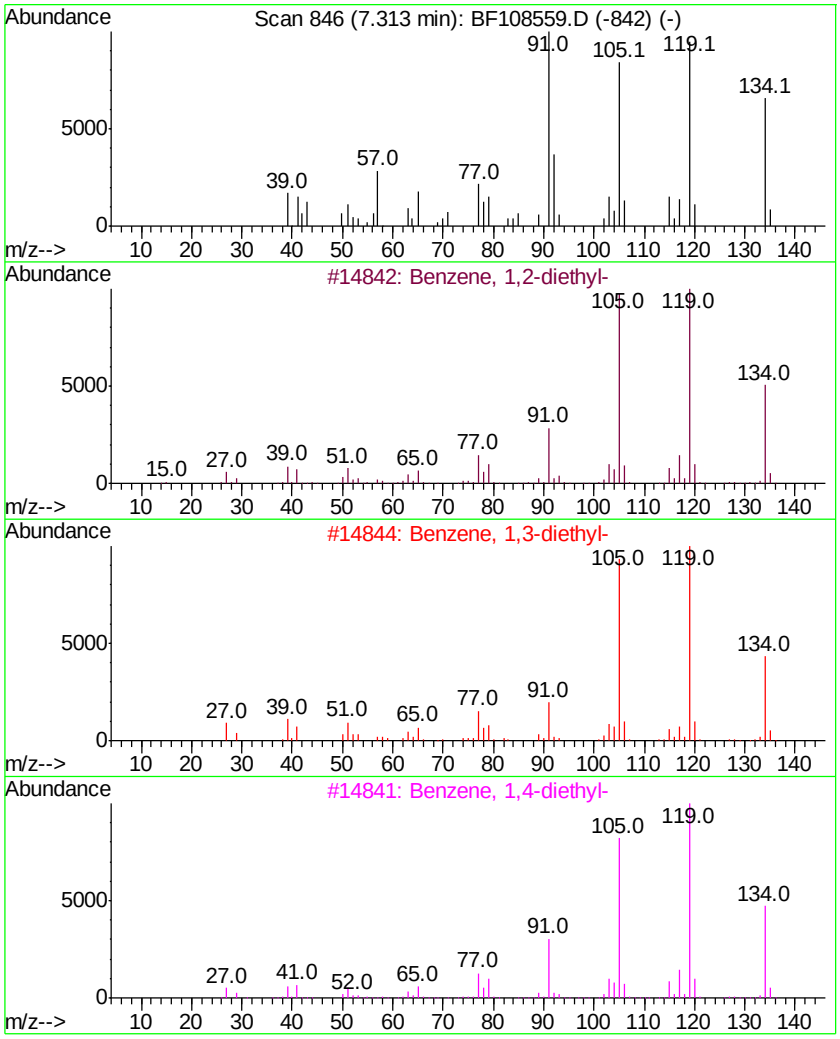
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

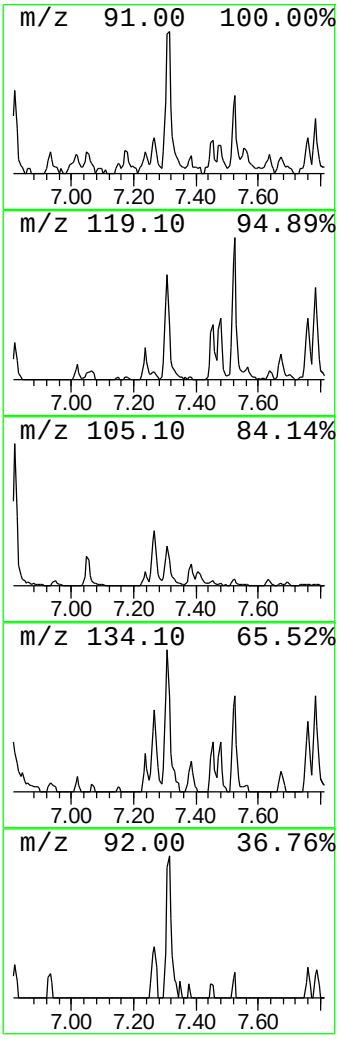
****

Peak Number 5 Benzene, 1,2-diethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.31	2.82 ng	103361	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
2	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	96
3	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	95
4	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	90
5	2,6-Dimethyl-1,3,5,7-octatetraen...	134	C10H14	000460-01-5	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082818\
Data File : BF108559.D
Acq On : 28 Aug 2018 16:58
Operator : JU/SJ
Sample : J4523-02 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

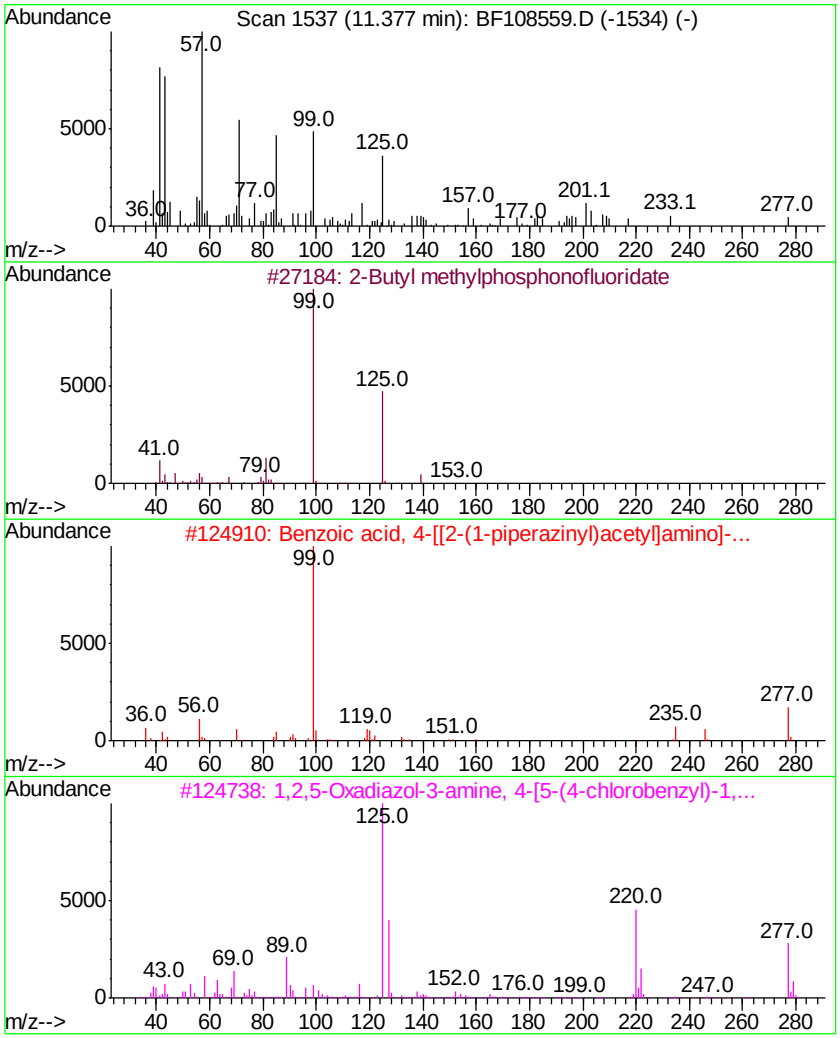
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

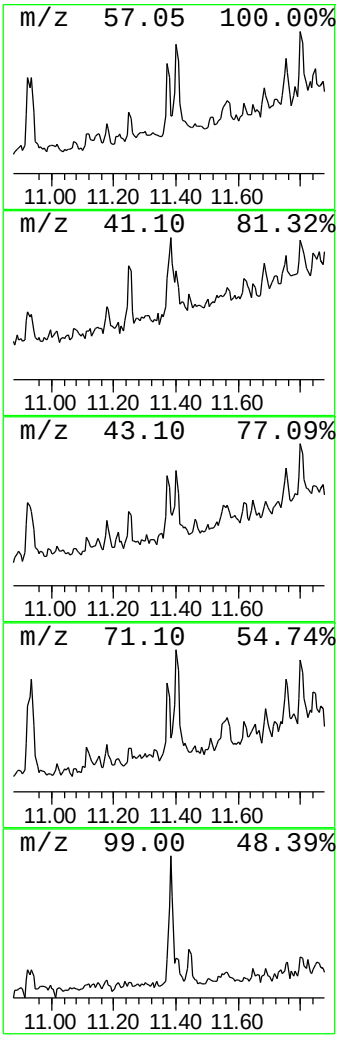
****

Peak Number 6 unknown11.38 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.38	2.53 ng	103832	Phenanthrene-d10	11.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butyl methylphosphonofluoridate	154	C5H12FO2P	000352-52-3	47
2	Benzoic acid, 4-[[2-(1-piperazin...	277	C14H19N3O3	1000350-32-6	22
3	1,2,5-Oxadiazol-3-amine, 4-[5-(4...	277	C11H8ClN5O2	1000276-59-0	22
4	6,7-Dihydro-5H-benzo[1,2,5]oxadi...	277	C13H12ClN3O2	1000301-42-2	16
5	Pyrazol-3-one, 5-amino-1-cyclohe...	195	C10H17N3O	1000316-44-6	14





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082818\
Data File : BF108559.D
Acq On : 28 Aug 2018 16:58
Operator : JU/SJ
Sample : J4523-02 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

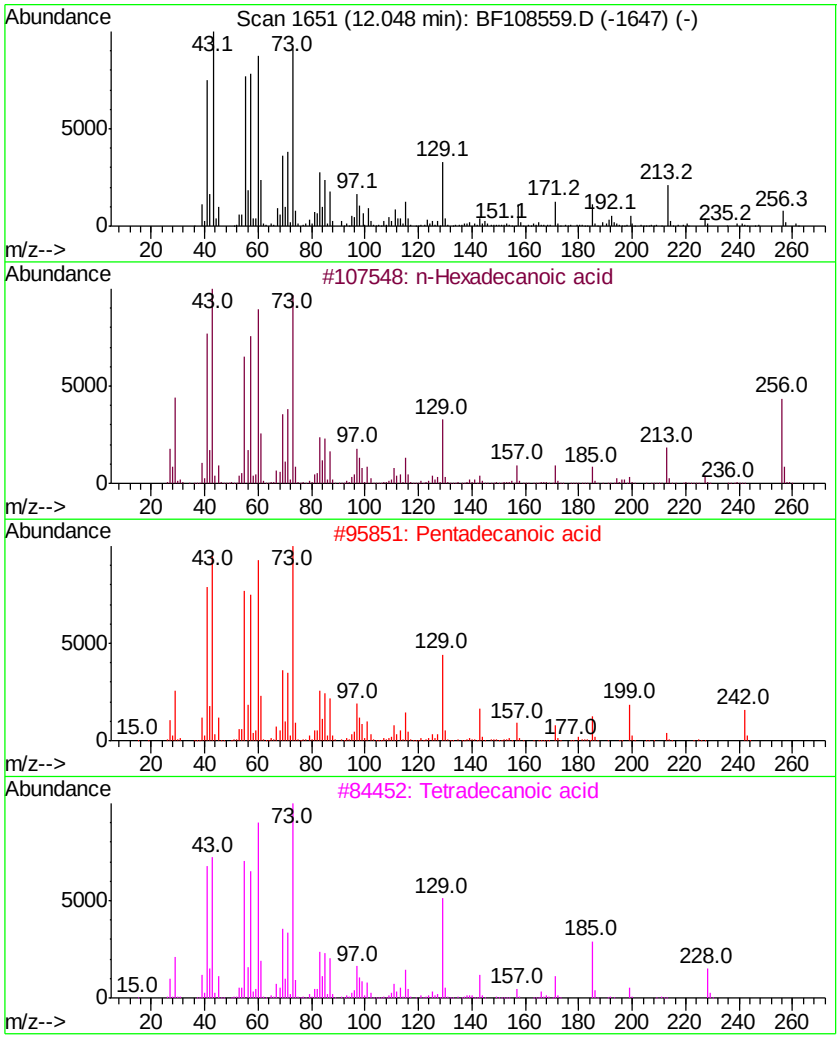
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

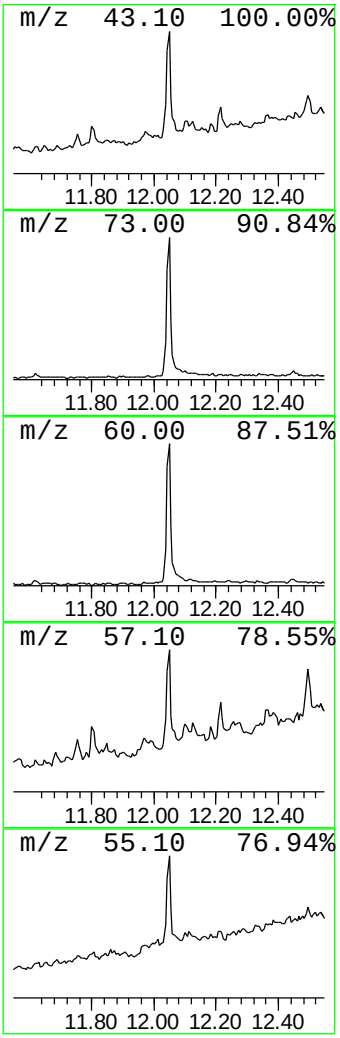
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	11.01 ng	450938	Phenanthrene-d10	11.54

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	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	70
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082818\
Data File : BF108559.D
Acq On : 28 Aug 2018 16:58
Operator : JU/SJ
Sample : J4523-02 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

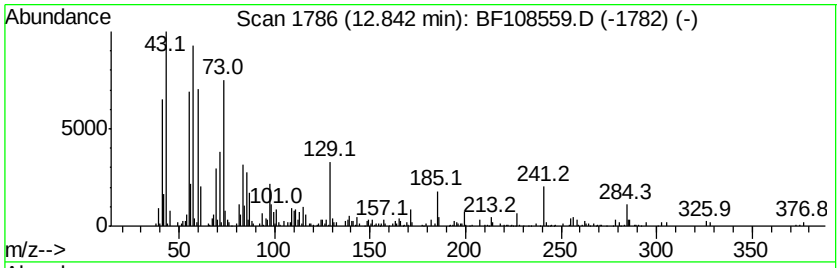
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

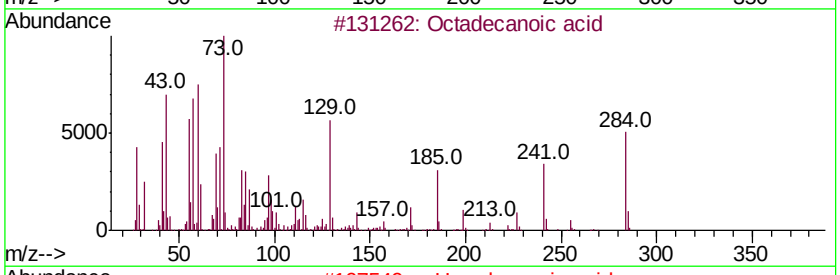
****

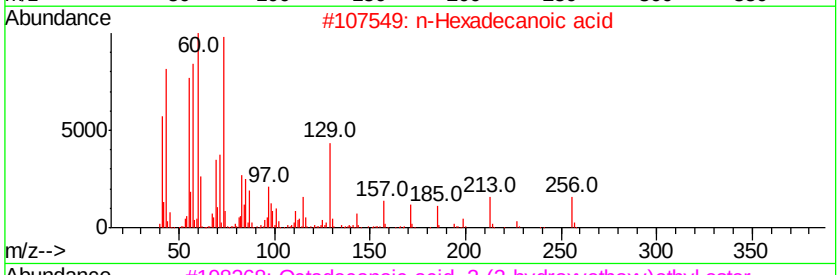
Peak Number 8 Octadecanoic acid Concentration Rank 5

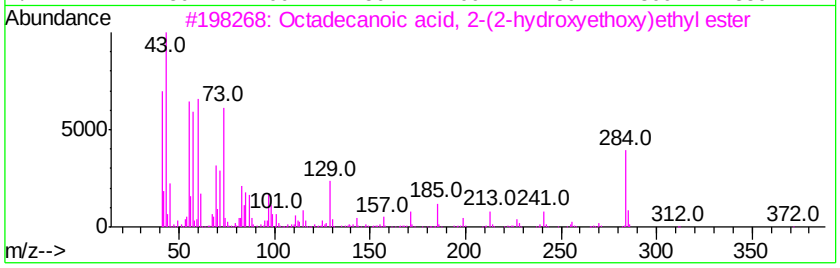
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	7.14 ng	292476	Phenanthrene-d10	11.54

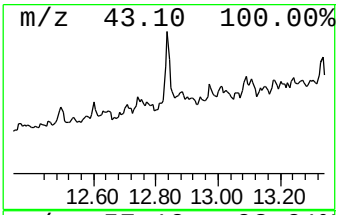
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72

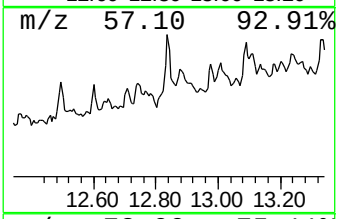


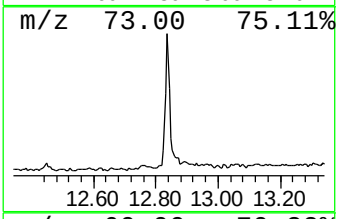


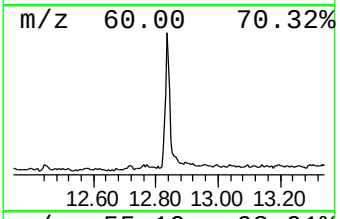


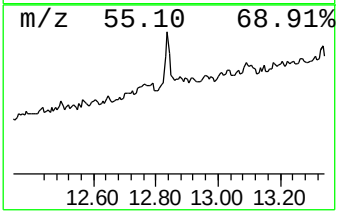












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082818\
Data File : BF108559.D
Acq On : 28 Aug 2018 16:58
Operator : JU/SJ
Sample : J4523-02 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

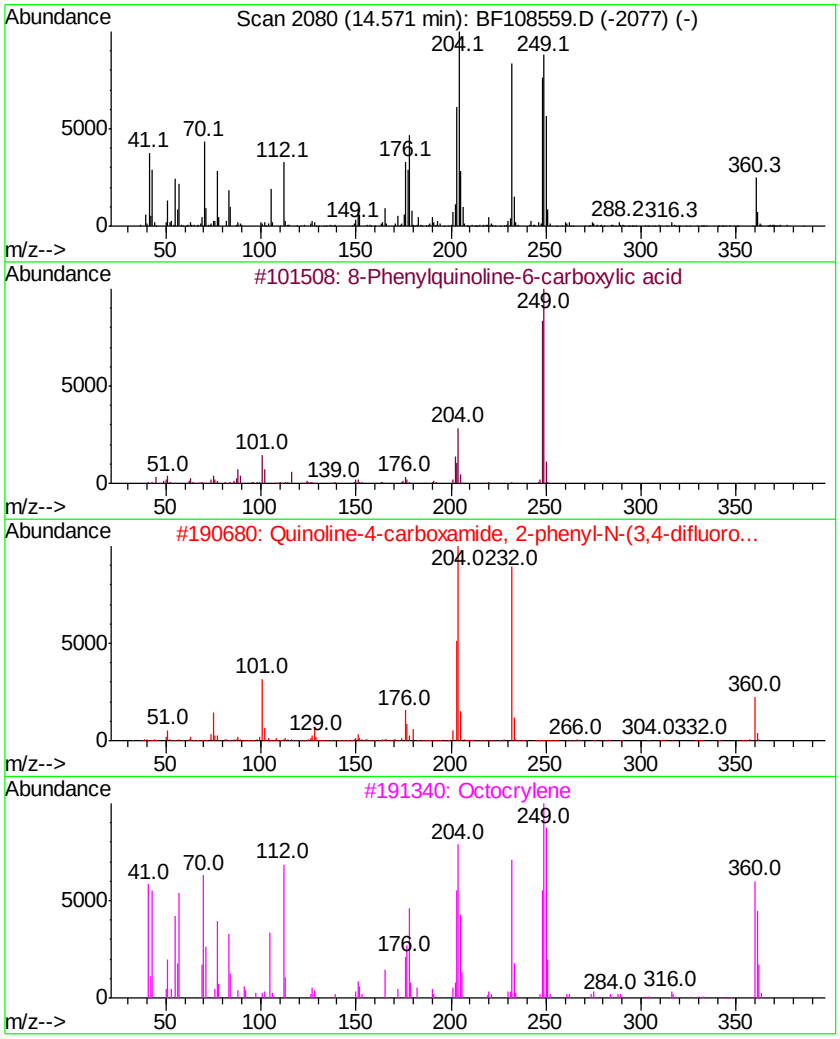
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

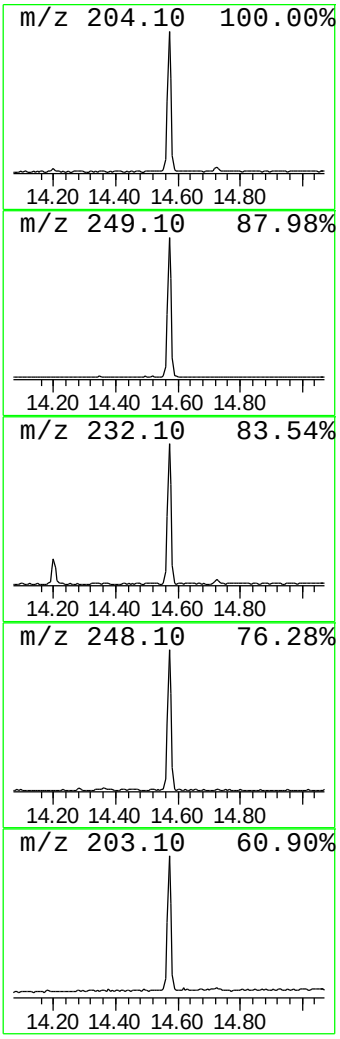
****

Peak Number 9 unknown14.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	28.96 ng	1028760	Chrysene-d12	14.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8-Phenylquinoline-6-carboxylic acid	249	C16H11NO2	035871-15-9	43
2	Quinoline-4-carboxamide, 2-phenyl...	360	C22H14F2N2O	303133-50-8	41
3	Octocrylene	361	C24H27NO2	006197-30-4	22
4	Phosphine, methyl-(2,4,6-triisop...	250	C16H27P	158748-69-7	20
5	2,5-Dimethyl-7,7,8,8-tetracyano-...	232	C14H8N4	001487-82-7	18





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082818\
Data File : BF108559.D
Acq On : 28 Aug 2018 16:58
Operator : JU/SJ
Sample : J4523-02 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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
Benzene, 1-ethyl-...	6.52	2.1	ng	76372	1	7.00	731952	20.0
unknown6.78	6.78	32.2	ng	1178430	1	7.00	731952	20.0
Benzene, 1,2,3-tr...	6.82	4.6	ng	168371	1	7.00	731952	20.0
Benzene, 1,2-diet...	7.31	2.8	ng	103361	1	7.00	731952	20.0
unknown11.38	11.38	2.5	ng	103832	4	11.54	819427	20.0
n-Hexadecanoic acid	12.05	11.0	ng	450938	4	11.54	819427	20.0
Octadecanoic acid	12.84	7.1	ng	292476	4	11.54	819427	20.0
unknown14.57	14.57	29.0	ng	1028760	5	14.20	710449	20.0