LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080923\
Data File : BF134687.D
Acq On : 09 Aug 2023 13:09
Operator : CG\JU
Sample : 03903-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-08

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-BF080123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134687.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.151	5	11	16	rBV	45972	66684	1.93%	0.213%
2	3.645	254	265	273	rBV3	19659	40404	1.17%	0.129%
3	5.028	496	500	505	rBV	89604	115326	3.34%	0.368%
4	5.292	542	545	550	rBV	163954	154442	4.48%	0.493%
5	5.398	559	563	565	rBV	246323	274519	7.96%	0.876%
6	5.428	565	568	572	rVB	2975965	3098541	89.83%	9.885%
7	5.975	652	661	664	rBV3	42171	55847	1.62%	0.178%
8	6.263	708	710	713	rVB	104007	81926	2.38%	0.261%
9	6.328	719	721	724	rBV	172241	157569	4.57%	0.503%
10	6.363	724	727	730	rVB	122733	102730	2.98%	0.328%
11	6.404	730	734	735	rBV2	124287	105767	3.07%	0.337%
12	6.439	735	740	742	rVV	3008598	3114028	90.28%	9.934%
13	6.486	742	748	754	rVB	73574	77150	2.24%	0.246%
14	6.628	769	772	779	rBV	496903	396242	11.49%	1.264%
15	6.804	798	802	805	rBV	1882313	1550025	44.94%	4.945%
16	6.857	808	811	819	rVB2	73623	78084	2.26%	0.249%
17	7.122	852	856	858	rBV	58589	51990	1.51%	0.166%
18	7.333	887	892	893	rBV	55096	47329	1.37%	0.151%
19	7.363	893	897	900	rVB	2340455	1979119	57.37%	6.314%
20	8.081	1015	1019	1022	rBV	2621397	2048828	59.40%	6.536%
21	8.145	1028	1030	1038	rVB	90156	85706	2.48%	0.273%
22	8.539	1095	1097	1103	rBV	43110	45723	1.33%	0.146%
23	9.157	1198	1202	1205	rBV	4226450	3449460	100.00%	11.004%
24	9.275	1219	1222	1226	rBV	154623	125094	3.63%	0.399%
25	9.598	1273	1277	1284	rBV	152073	144852	4.20%	0.462%
26	9.833	1314	1317	1321	rBV	2388816	2156483	62.52%	6.879%
27	10.627	1447	1452	1455	rBV	2010949	1919026	55.63%	6.122%
28	10.751	1470	1473	1481	rBV3	53269	106393	3.08%	0.339%
29	10.957	1503	1508	1512	rBV4	44751	85796	2.49%	0.274%
30	11.198	1546	1549	1551	rBV2	60420	45904	1.33%	0.146%
31	11.227	1551	1554	1557	rVB2	71492	70849	2.05%	0.226%
32	11.327	1567	1571	1574	rBV	2116318	1853611	53.74%	5.913%
33	11.369	1576	1578	1581	rBV3	28439	42642	1.24%	0.136%
34	11.445	1589	1591	1596	rBV3	35385	42424	1.23%	0.135%
35	11.510	1600	1602	1604	rBV3	46609	54512	1.58%	0.174%
36	11.580	1612	1614	1617	rVB	44795	41523	1.20%	0.132%

LSC Area Percent Report

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Misc :
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Instrument :
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Integration Parameters: rteint.p
Integrator: RTE
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Start Thrs: 0.2 Max Peaks: 100
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.627	1620	1622	1625	rBV	50485	49811	1.44%	0.159%
38	11.669	1625	1629	1632	rBV3	78145	125692	3.64%	0.401%
39	11.792	1647	1650	1653	rBV3	43523	50311	1.46%	0.160%
40	11.863	1658	1662	1665	rBV2	360427	335081	9.71%	1.069%
41	12.039	1689	1692	1694	rBV3	56134	62392	1.81%	0.199%
42	12.321	1735	1740	1744	rBV3	101452	176779	5.12%	0.564%
43	12.380	1748	1750	1753	rBV2	101681	93579	2.71%	0.299%
44	12.463	1762	1764	1768	rBV5	64246	77079	2.23%	0.246%
45	12.539	1774	1777	1780	rBV	166128	164525	4.77%	0.525%
46	12.768	1814	1816	1819	rBV	169368	158699	4.60%	0.506%
47	12.833	1824	1827	1830	rBV	135966	143005	4.15%	0.456%
48	12.921	1838	1842	1845	rBV	2811353	2612108	75.73%	8.333%
49	13.710	1974	1976	1979	rBV2	189244	226975	6.58%	0.724%
50	13.974	2017	2021	2025	rBV2	1530053	1821630	52.81%	5.811%
51	14.621	2129	2131	2136	rVB	334564	341656	9.90%	1.090%
52	15.456	2269	2273	2276	rBV	926463	1041207	30.18%	3.322%

Sum of corrected areas: 31347077

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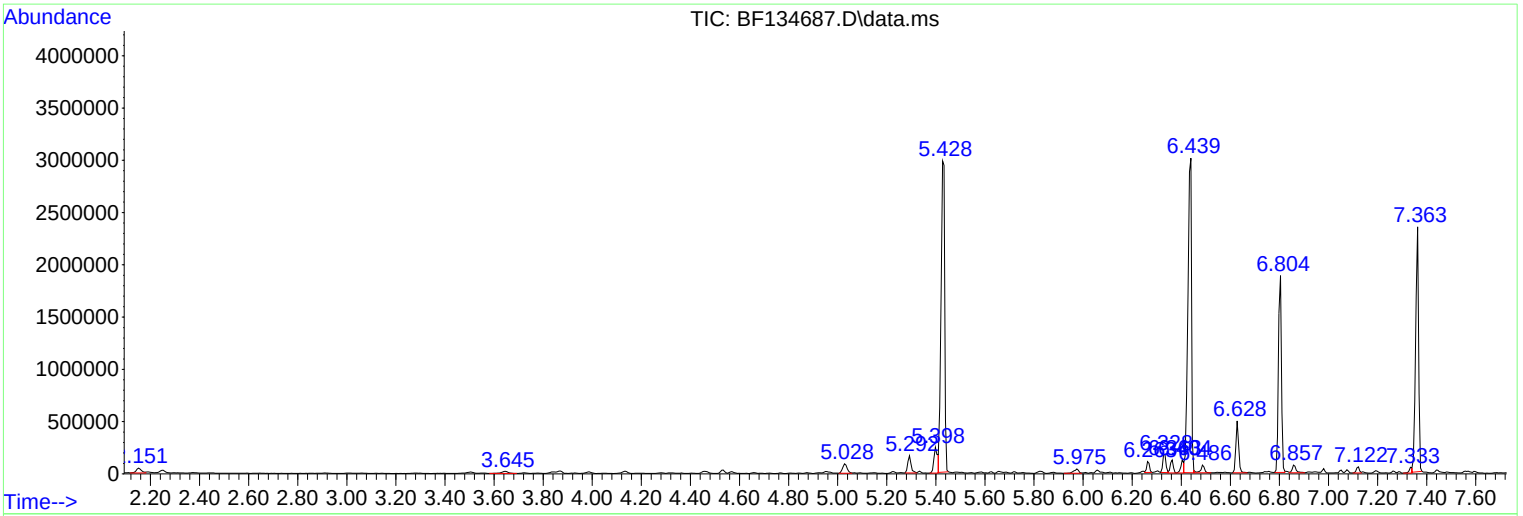
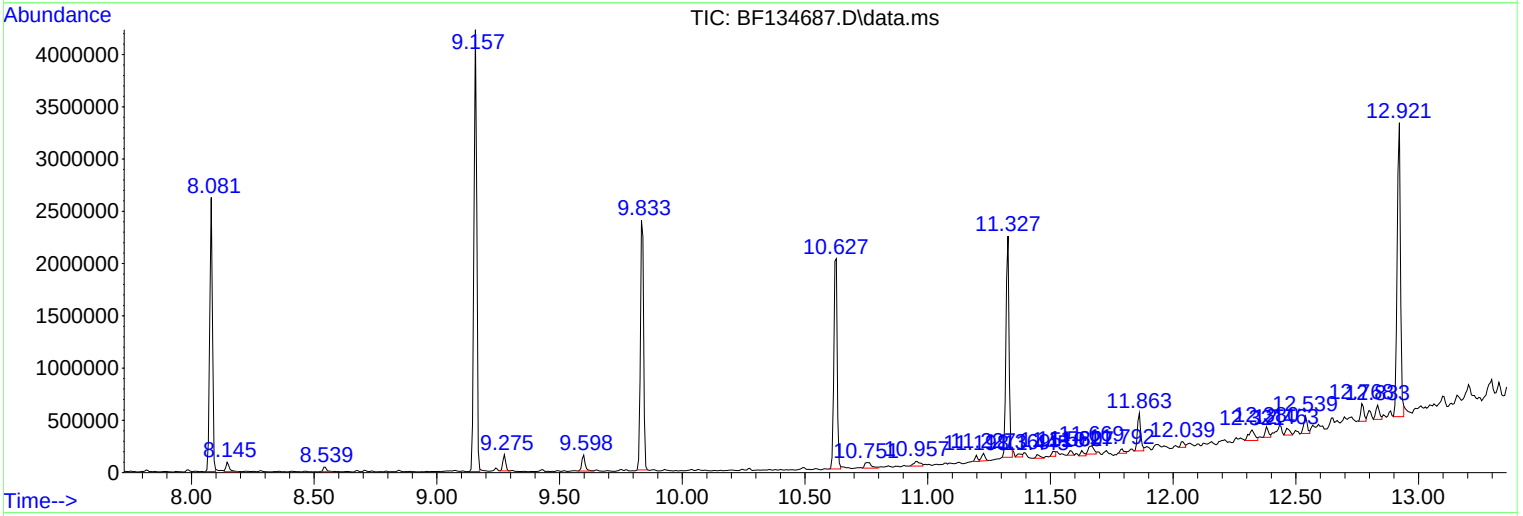
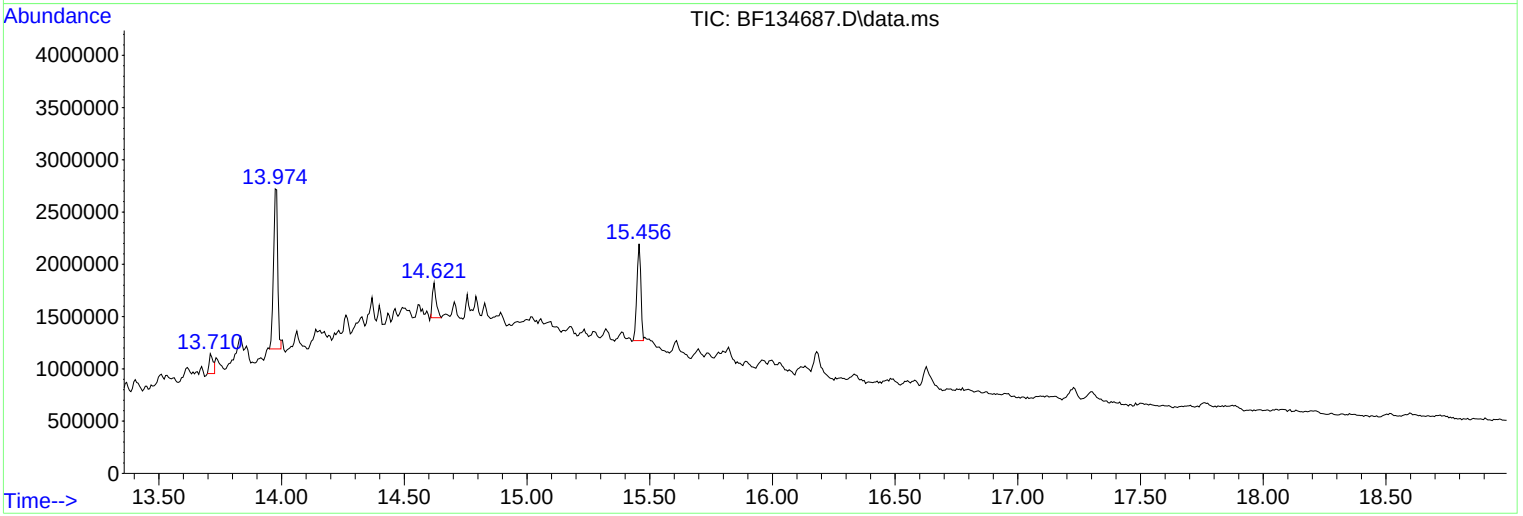
Instrument :
BNA_F
ClientSampleId :
MW-08

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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 : BF134687.D
Acq On : 09 Aug 2023 13:09
Operator : CG\JU
Sample : 03903-08
Misc :
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Instrument :
BNA_F
ClientSampleId :
MW-08

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

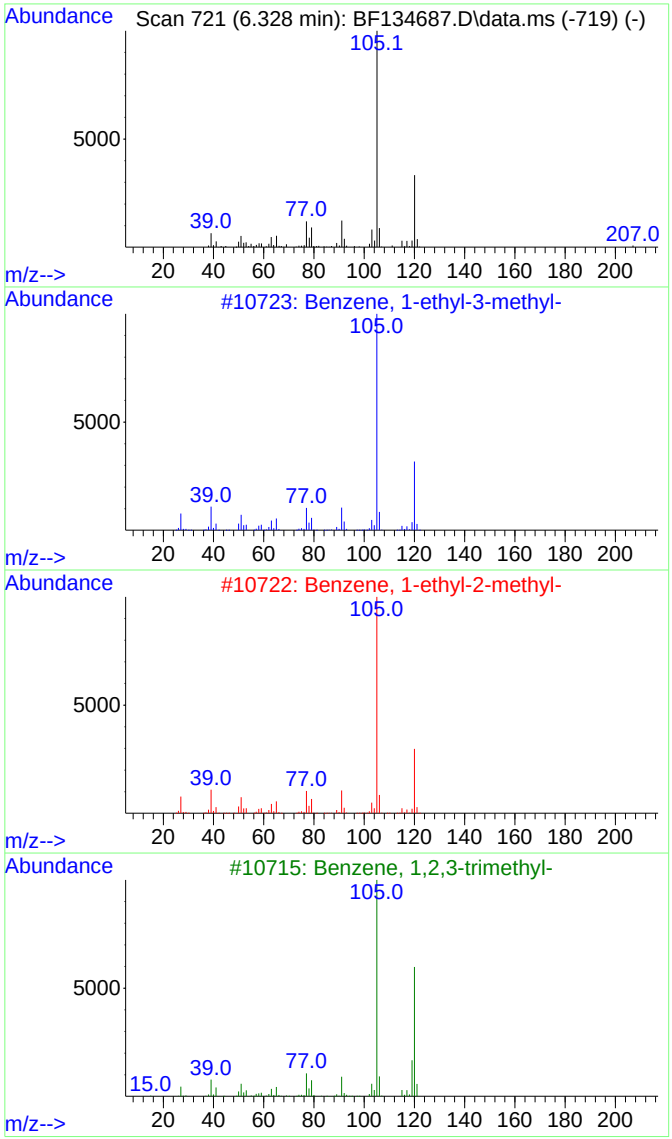
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

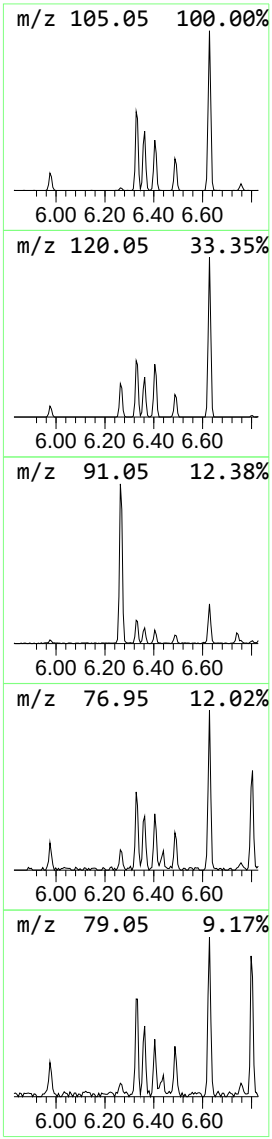
****

Peak Number 1 Benzene, 1-ethyl-3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.328	2.03 ng	157569	1,4-Dichlorobenzene-d4	6.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





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Sample : 03903-08
Misc :
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Instrument :
BNA_F
ClientSampleId :
MW-08

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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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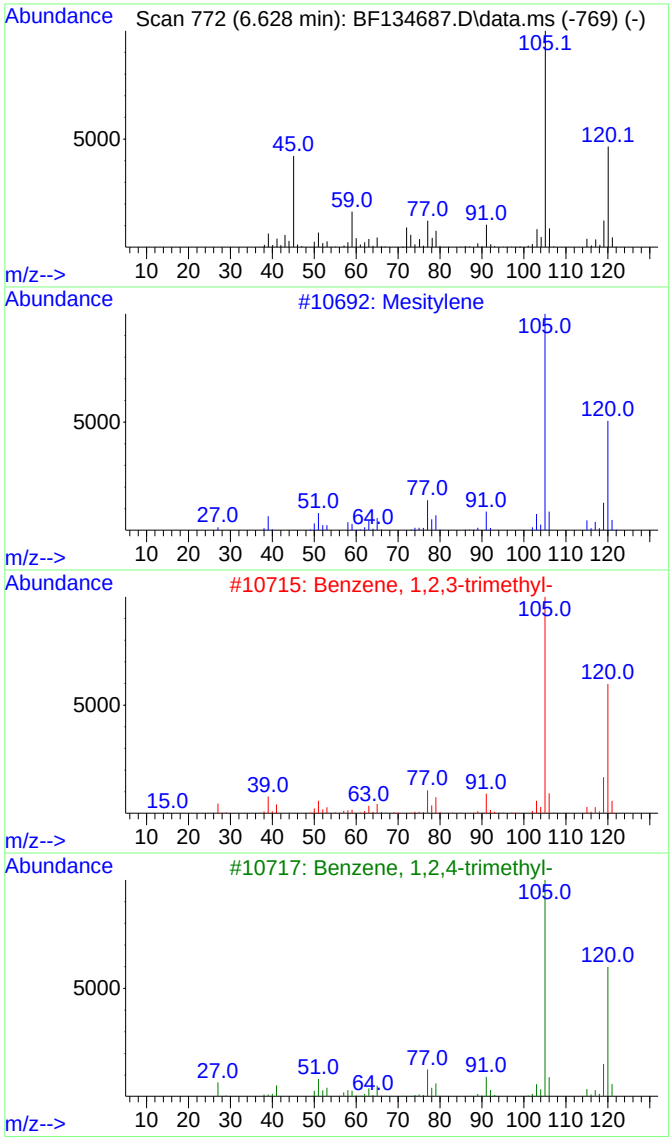
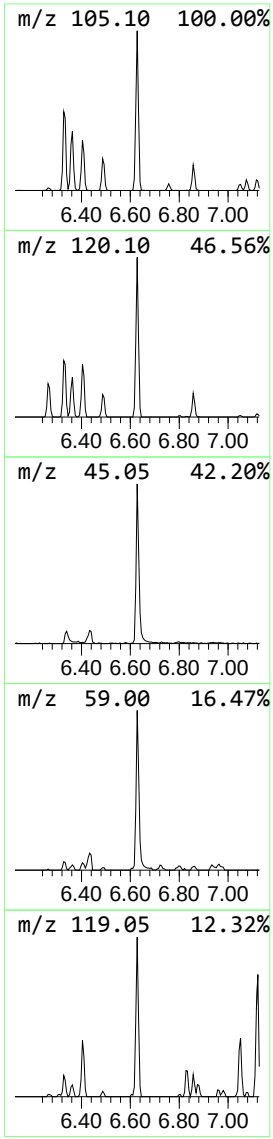
Peak Number 2 Mesitylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.628	5.11 ng	396242	1,4-Dichlorobenzene-d4	6.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylene	120	C9H12	000108-67-8	92
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	92
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	60
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	55





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Operator : CG\JU
Sample : 03903-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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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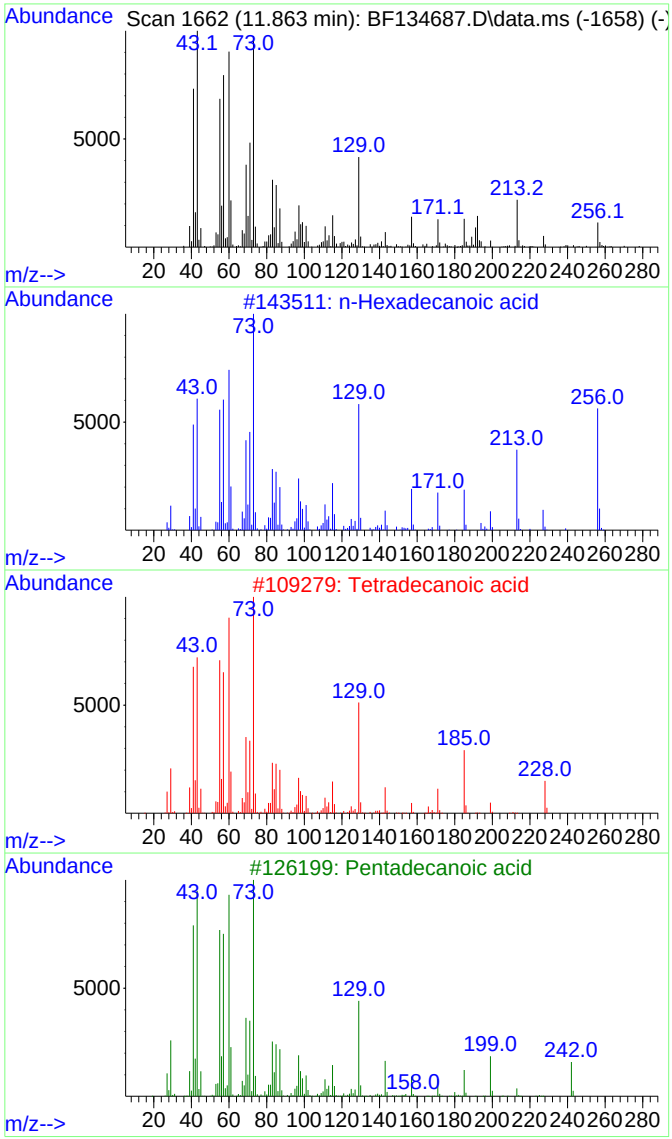
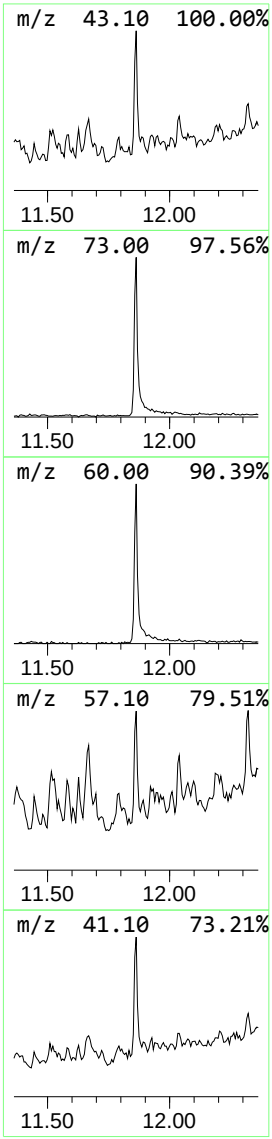
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	3.62 ng	335081	Phenanthrene-d10	11.327

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Tridecanoic acid	214	C13H26O2	000638-53-9	68





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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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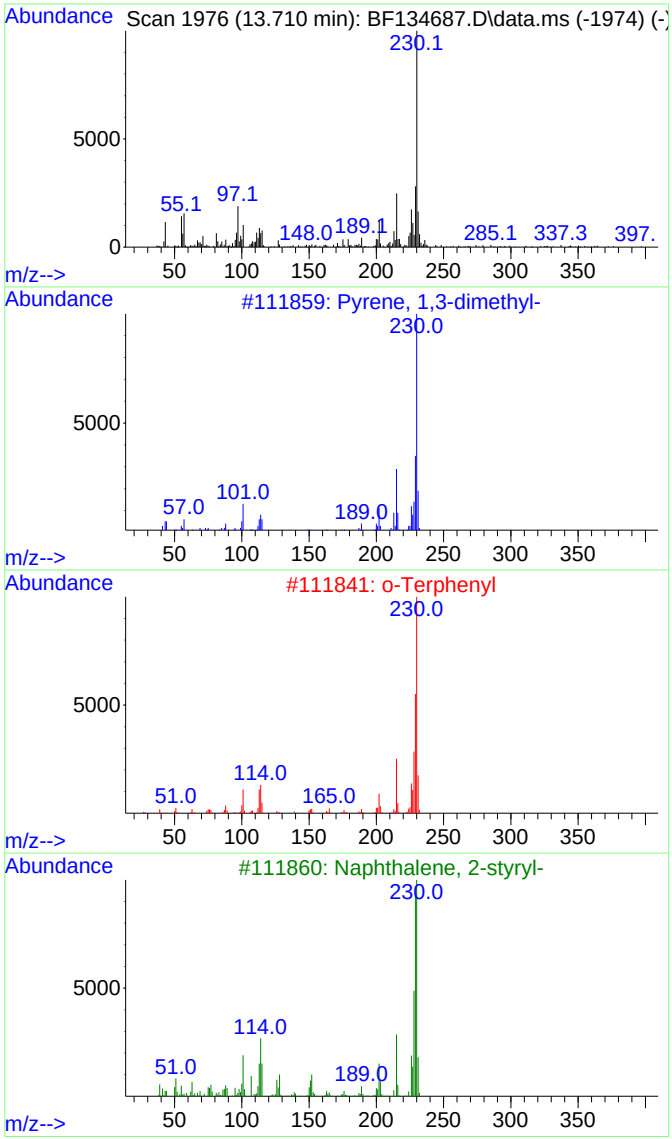
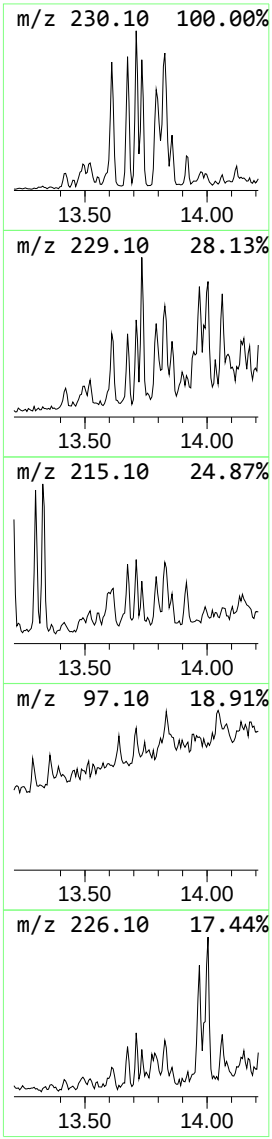
Peak Number 4 Pyrene, 1,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.710	2.49 ng	226975	Chrysene-d12	13.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1,3-dimethyl-	230	C18H14	064401-21-4	93
2	o-Terphenyl	230	C18H14	000084-15-1	81
3	Naphthalene, 2-styryl-	230	C18H14	002039-70-5	81
4	5,6-Dihydrochrysene	230	C18H14	002091-92-1	68
5	(6,7-Dimethoxy-3,4-dihydro-1-iso...	230	C13H14N2O2	1000332-51-4	59





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Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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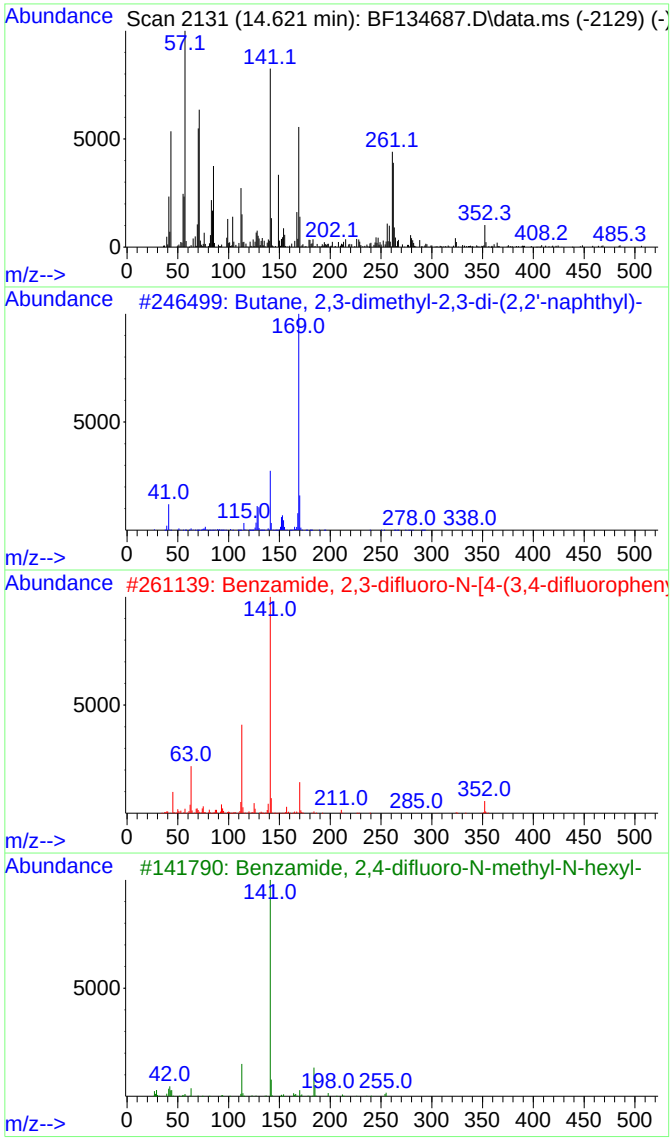
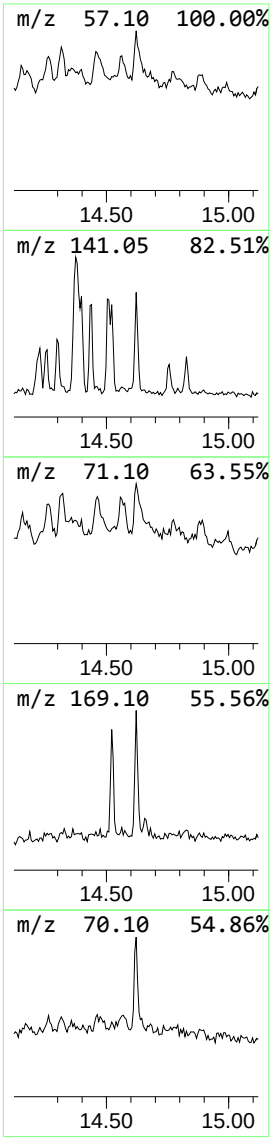
Peak Number 5 unknown14.621 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.621	3.75 ng	341656	Chrysene-d12	13.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-2,3-di-(2,2...	338	C26H26	1000150-93-8	35
2	Benzamide, 2,3-difluoro-N-[4-(3,...	352	C16H8F4N2OS	1000277-49-1	22
3	Benzamide, 2,4-difluoro-N-methyl...	255	C14H19F2NO	1000437-06-3	20
4	Benzoic acid, 2,6-difluoro-, 2-a...	276	C15H10F2O3	1000266-38-6	18
5	Benzamide, 2,6-difluoro-N-methyl...	255	C14H19F2NO	1000421-47-6	18





Tentatively Identified Compound (LSC) summary

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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-ethy...	6.328	2.0	ng	157569	1	6.804	1550030	20.0
Mesitylene	6.628	5.1	ng	396242	1	6.804	1550030	20.0
n-Hexadecanoic ...	11.863	3.6	ng	335081	4	11.327	1853610	20.0
Pyrene, 1,3-dim...	13.710	2.5	ng	226975	5	13.980	1821630	20.0
unknown14.621	14.621	3.8	ng	341656	5	13.980	1821630	20.0