LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
Data File : BF136368.D
Acq On : 02 Dec 2023 08:54
Operator : CG\JU
Sample : 05420-01
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-12018

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-BF112723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136368.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.699	269	274	279	rBV2	15004	24218	1.33%	0.140%
2	3.905	305	309	315	rVB2	16162	22270	1.23%	0.129%
3	5.040	499	502	507	rVB	66592	72949	4.01%	0.422%
4	5.240	532	536	545	rVB	55647	60746	3.34%	0.351%
5	5.440	566	570	573	rBV	1971222	1817052	100.00%	10.510%
6	6.093	677	681	684	rVB	615013	499249	27.48%	2.888%
7	6.257	703	709	713	rBV2	56047	48959	2.69%	0.283%
8	6.440	735	740	743	rBV	1889282	1656140	91.14%	9.579%
9	6.510	748	752	755	rVV	247377	199985	11.01%	1.157%
10	6.557	757	760	765	rVB2	27414	23655	1.30%	0.137%
11	6.640	771	774	785	rBV2	24713	45034	2.48%	0.260%
12	6.757	791	794	797	rVB	46409	35017	1.93%	0.203%
13	6.804	799	802	806	rBV	770741	598132	32.92%	3.460%
14	6.922	819	822	824	rBV	23704	20537	1.13%	0.119%
15	7.363	892	897	900	rBV	1282998	1104925	60.81%	6.391%
16	8.081	1015	1019	1022	rBV	789723	642359	35.35%	3.715%
17	9.157	1198	1202	1205	rBV	1901190	1498077	82.45%	8.665%
18	9.281	1219	1223	1228	rVB	32600	32884	1.81%	0.190%
19	9.492	1257	1259	1263	rVB2	27266	23743	1.31%	0.137%
20	9.839	1314	1318	1321	rBV	702251	549646	30.25%	3.179%
21	10.628	1448	1452	1465	rVB	889889	775571	42.68%	4.486%
22	11.328	1568	1571	1574	rBV	698890	597548	32.89%	3.456%
23	11.351	1574	1575	1579	rVV	136851	93579	5.15%	0.541%
24	11.404	1579	1584	1588	rVB	32957	31982	1.76%	0.185%
25	11.833	1654	1657	1659	rBV	23567	20521	1.13%	0.119%
26	11.869	1659	1663	1667	rVV	153710	151804	8.35%	0.878%
27	11.945	1673	1676	1678	rBV	25135	24973	1.37%	0.144%
28	12.222	1720	1723	1726	rVB4	35722	30696	1.69%	0.178%
29	12.433	1753	1759	1775	rBV5	223226	803483	44.22%	4.647%
30	12.545	1775	1778	1783	rVB	263398	233892	12.87%	1.353%
31	12.657	1794	1797	1802	rBV3	56213	69744	3.84%	0.403%
32	12.704	1803	1805	1810	rVV6	24747	29355	1.62%	0.170%
33	12.775	1812	1817	1821	rVV	216861	242258	13.33%	1.401%
34	12.827	1824	1826	1832	rVB3	26131	31478	1.73%	0.182%
35	12.927	1839	1843	1846	rBV	1949497	1596056	87.84%	9.232%
36	12.992	1851	1854	1860	rVB3	20852	33445	1.84%	0.193%

LSC Area Percent Report

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Instrument :
BNA_F
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72-12018

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.110	1867	1874	1880	rVB2	42218	79977	4.40%	0.463%
38	13.175	1880	1885	1888	rBV2	33709	48999	2.70%	0.283%
39	13.210	1888	1891	1893	rBV2	28311	32256	1.78%	0.187%
40	13.233	1893	1895	1900	rVB6	31932	34754	1.91%	0.201%
41	13.304	1904	1907	1910	rBV3	26039	23602	1.30%	0.137%
42	13.339	1910	1913	1915	rBV4	18706	20004	1.10%	0.116%
43	13.451	1928	1932	1934	rBV2	90075	95898	5.28%	0.555%
44	13.474	1934	1936	1939	rVV	78225	74291	4.09%	0.430%
45	13.510	1939	1942	1944	rVV2	44124	47239	2.60%	0.273%
46	13.533	1944	1946	1952	rVB5	57817	64215	3.53%	0.371%
47	13.616	1957	1960	1966	rVB	26099	43459	2.39%	0.251%
48	13.692	1970	1973	1976	rBV5	26027	27234	1.50%	0.158%
49	13.780	1986	1988	1994	rVV3	29112	34515	1.90%	0.200%
50	13.845	1996	1999	2003	rVB	51683	54956	3.02%	0.318%
51	13.927	2009	2013	2017	rBV7	26640	61414	3.38%	0.355%
52	13.974	2017	2021	2025	rVV2	1242314	1511910	83.21%	8.745%
53	14.010	2025	2027	2030	rVB	117785	93044	5.12%	0.538%
54	14.086	2038	2040	2044	rBV2	21877	20396	1.12%	0.118%
55	14.163	2050	2053	2056	rVB	39070	37303	2.05%	0.216%
56	14.210	2058	2061	2068	rVV6	146205	163507	9.00%	0.946%
57	14.469	2102	2105	2108	rVB	69441	65639	3.61%	0.380%
58	14.780	2155	2158	2160	rBV	37560	31540	1.74%	0.182%
59	15.033	2197	2201	2204	rBV	95063	157821	8.69%	0.913%
60	15.127	2214	2217	2221	rVB2	47765	59509	3.28%	0.344%
61	15.339	2250	2253	2259	rVB	41277	55790	3.07%	0.323%
62	15.398	2260	2263	2269	rVB	61806	76635	4.22%	0.443%
63	15.468	2270	2275	2281	rBV	364144	473124	26.04%	2.737%
64	15.974	2358	2361	2368	rVB3	36518	58193	3.20%	0.337%

Sum of corrected areas: 17289186

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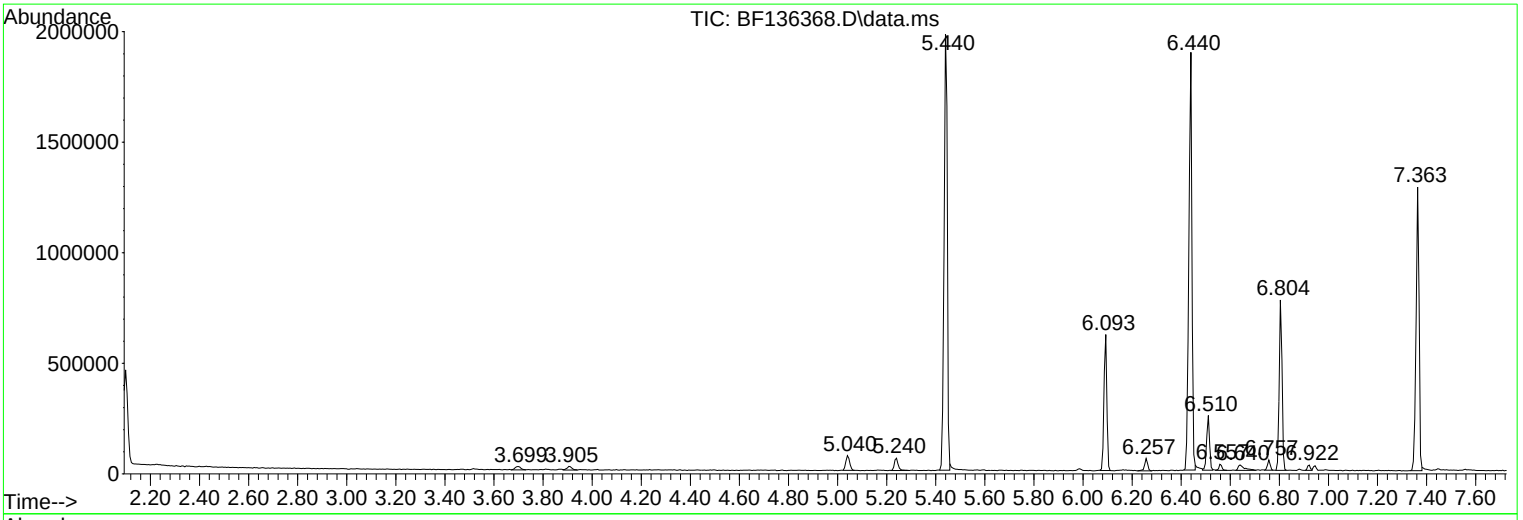
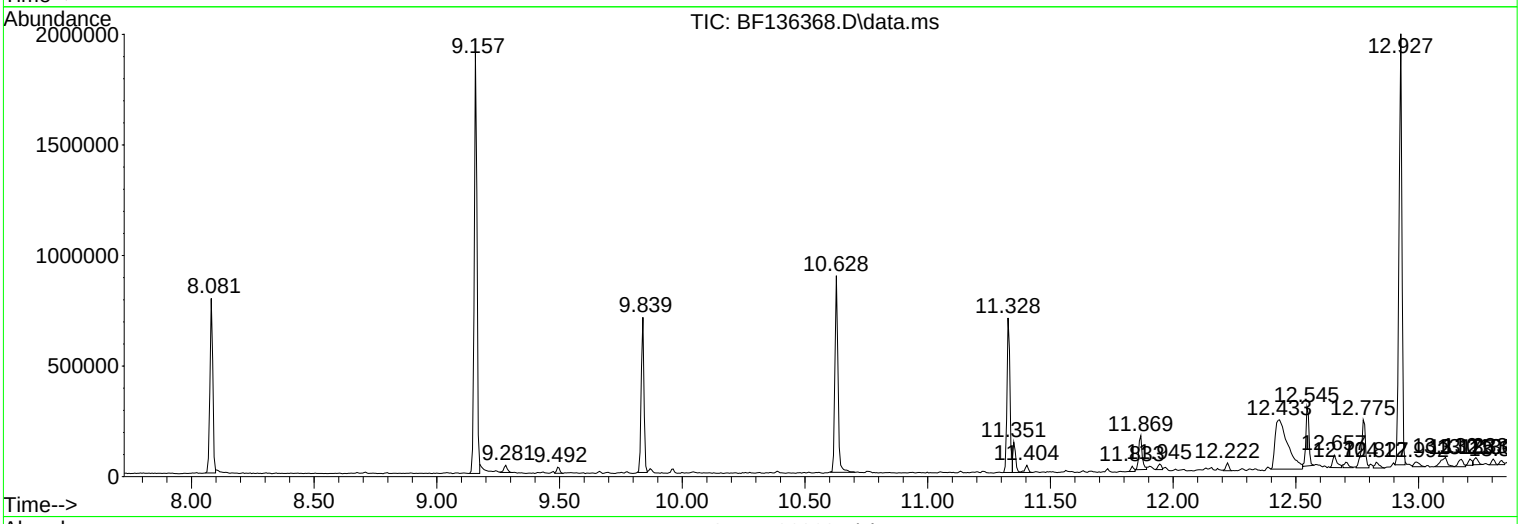
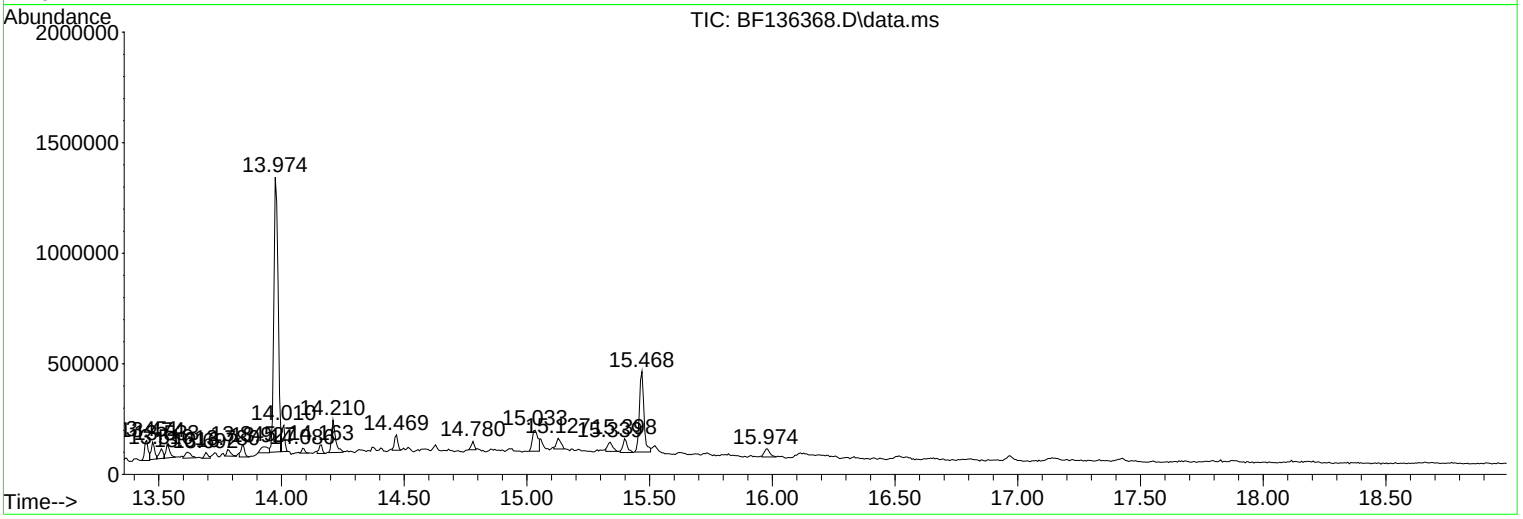
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

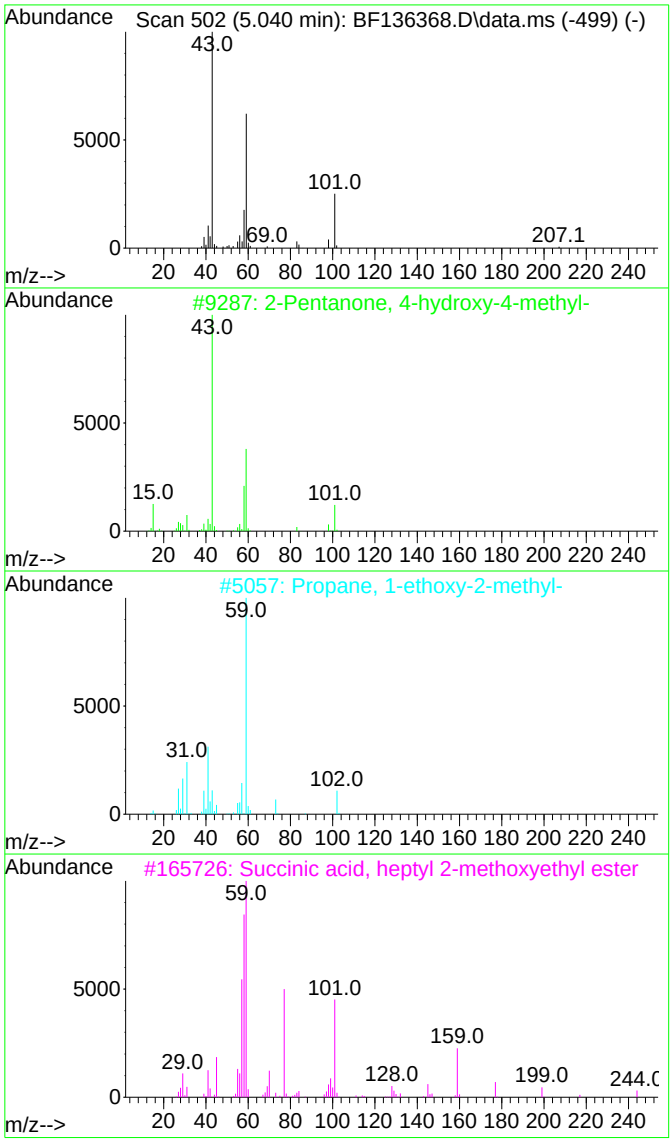
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

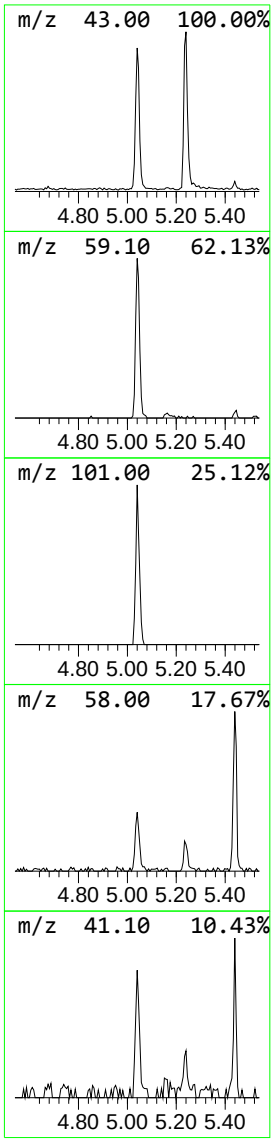
****

Peak Number 1 unknown5.040 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	2.44 ng	72949	1,4-Dichlorobenzene-d4	6.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	35
3	Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	28
4	Acetic acid, chloro-, 1,1-dimeth...	150	C6H11ClO2	000107-59-5	17
5	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	17





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Instrument :
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ClientSampleId :
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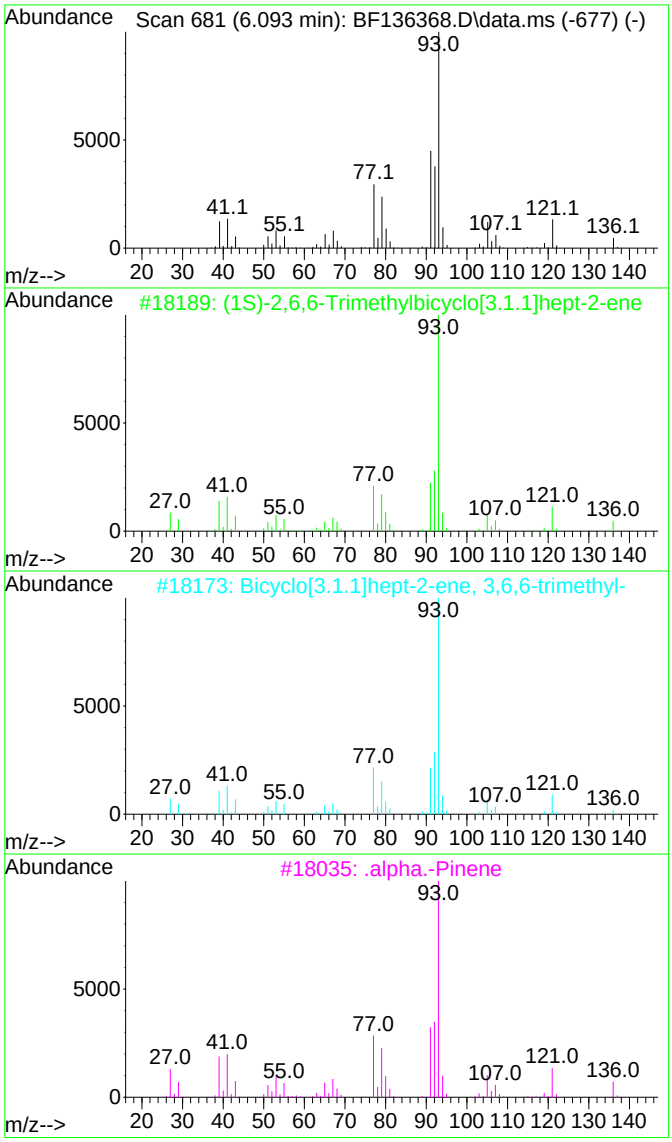
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

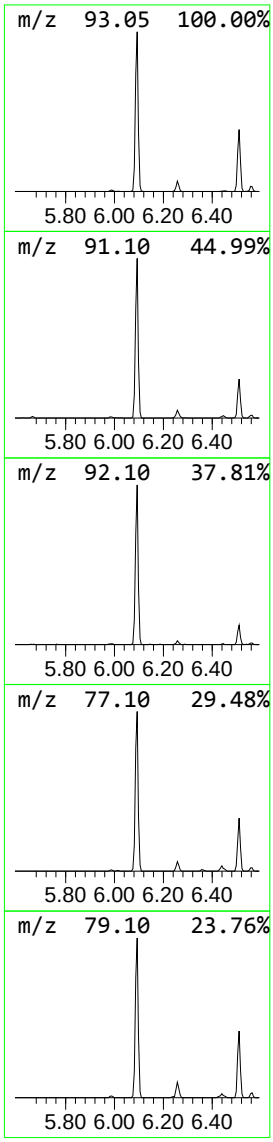
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (1S)-2,6,6-Trimethylbicyclo... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.093	16.69 ng	499249	1,4-Dichlorobenzene-d4	6.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	96
2	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	94
3	.alpha.-Pinene	136	C10H16	000080-56-8	94
4	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91
5	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	91





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

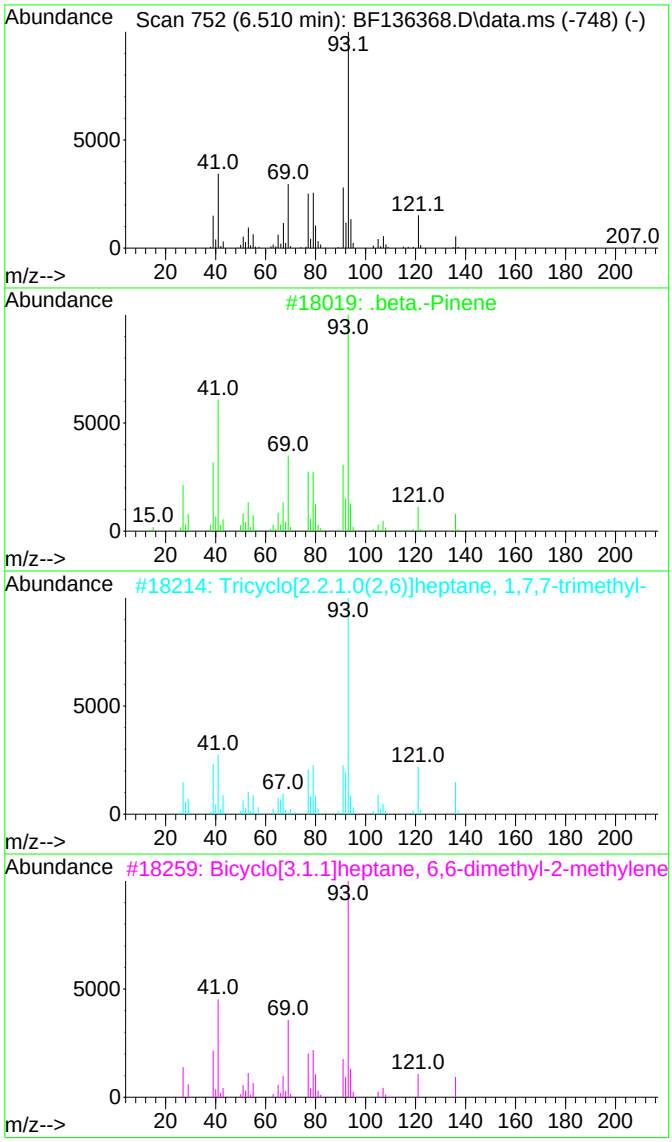
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

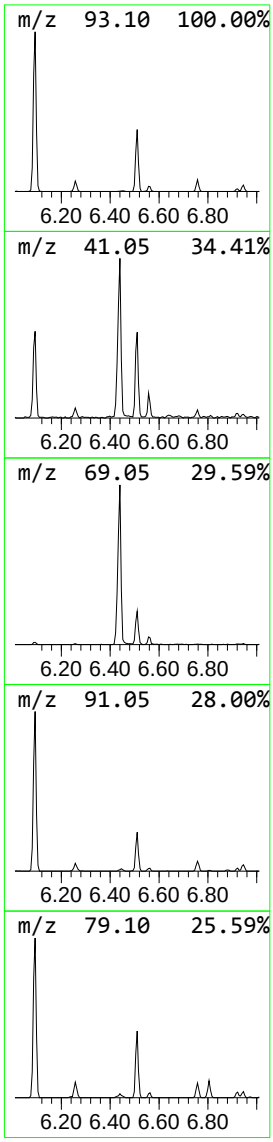
****

Peak Number 4 .beta.-Pinene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.510	6.69 ng	199985	1,4-Dichlorobenzene-d4	6.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Pinene	136	C10H16	000127-91-3	96
2	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91
3	Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	91
4	Bicyclo[3.1.0]hexane, 4-methylen...	136	C10H16	003387-41-5	87
5	Cyclohexane, 1-methylene-4-(1-me...	136	C10H16	000499-97-8	87





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TIC Library : C:\Database\NIST20.L
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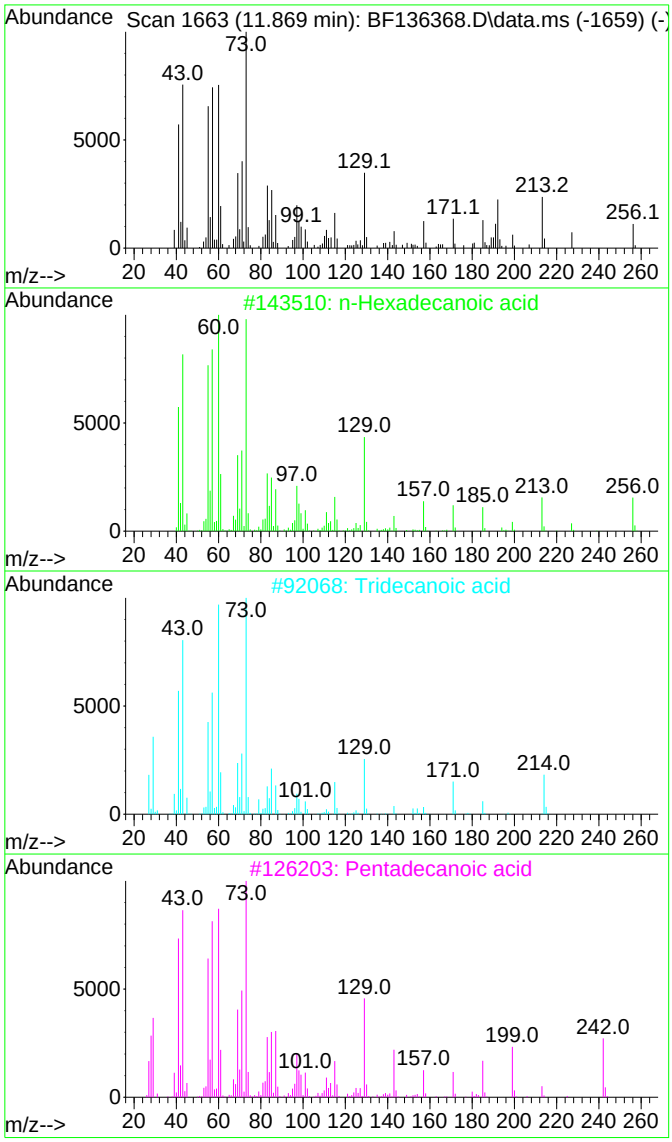
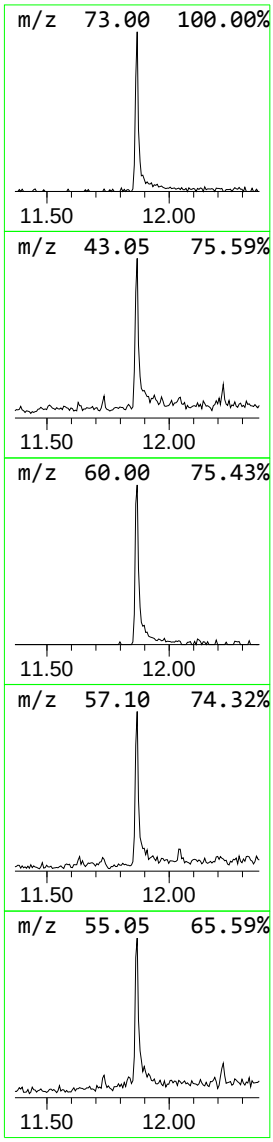
Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.869	5.08 ng	151804	Phenanthrene-d10	11.328

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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





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

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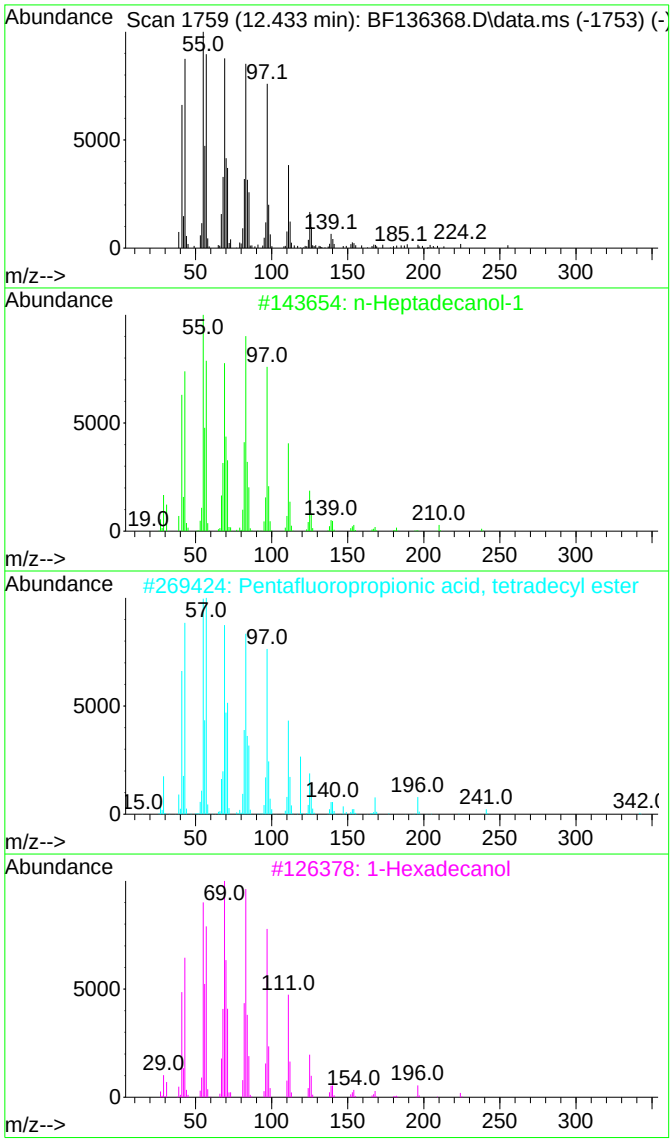
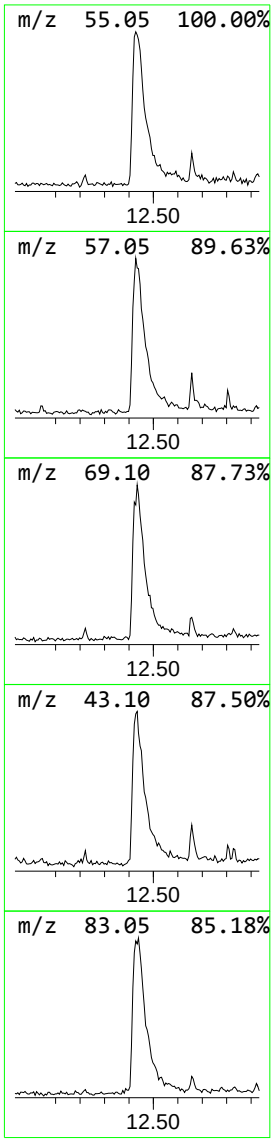
Peak Number 6 n-Heptadecanol-1 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.433	26.89 ng	803483	Phenanthrene-d10	11.328

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Heptadecanol-1	256	C17H36O	001454-85-9	95
2	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94
3	1-Hexadecanol	242	C16H34O	036653-82-4	94
4	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	94
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94





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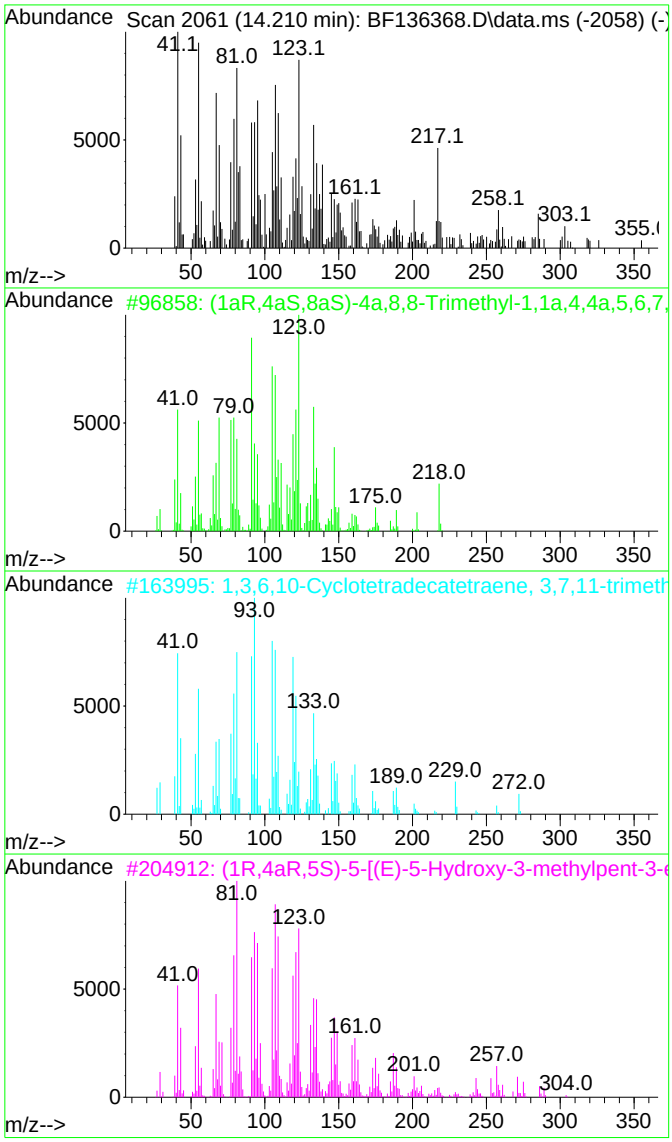
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

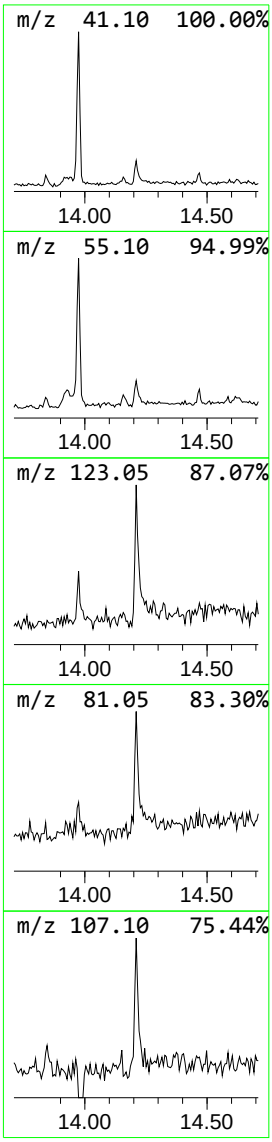
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (1aR,4aS,8aS)-4a,8,8-Trimet... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.210	2.16 ng	163507	Chrysene-d12	13.986

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1aR,4aS,8aS)-4a,8,8-Trimethyl-1...	218	C15H22O	000470-41-7	86
2	1,3,6,10-Cyclotetradecatetraene,...	272	C20H32	001898-13-1	70
3	(1R,4aR,5S)-5-[(E)-5-Hydroxy-3-m...	304	C20H32O2	1214984-94-7	68
4	Cyclopropanecarboxamide, 2,2-dim...	257	C17H23NO	339292-32-9	60
5	Bicyclo[5.2.0]nonane, 4-methylen...	204	C15H24	1000159-38-2	55





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TIC Library : C:\Database\NIST20.L
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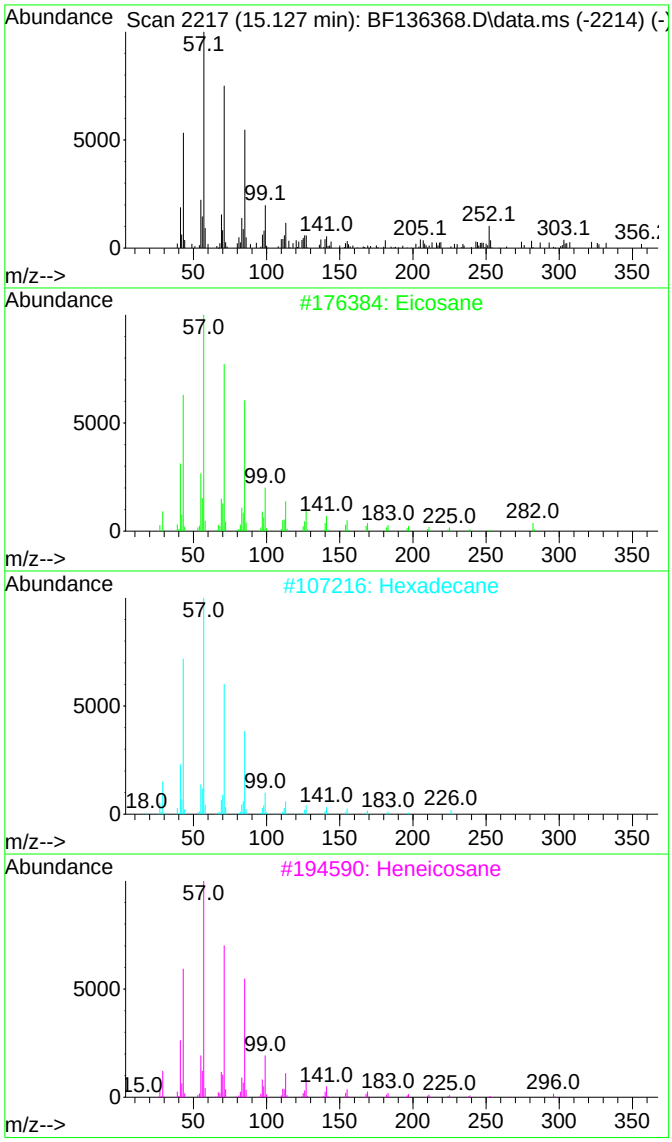
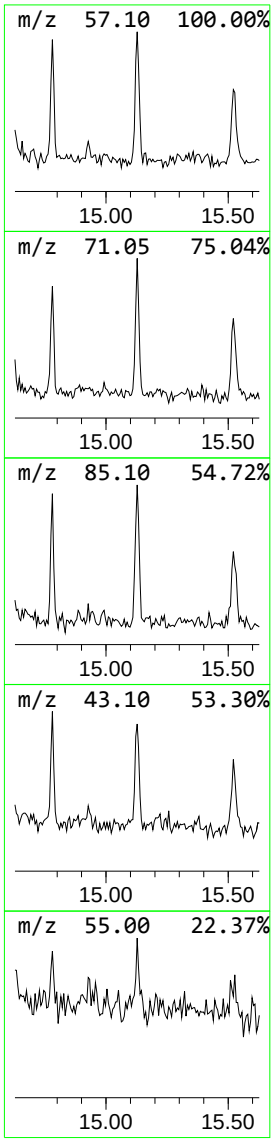
Peak Number 8 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	2.52 ng	59509	Perylene-d12	15.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Hexadecane	226	C16H34	000544-76-3	90
3	Heneicosane	296	C21H44	000629-94-7	87
4	Heptadecane	240	C17H36	000629-78-7	83
5	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	83





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Operator : CG\JU
Sample : 05420-01
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
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ClientSampleId :
72-12018

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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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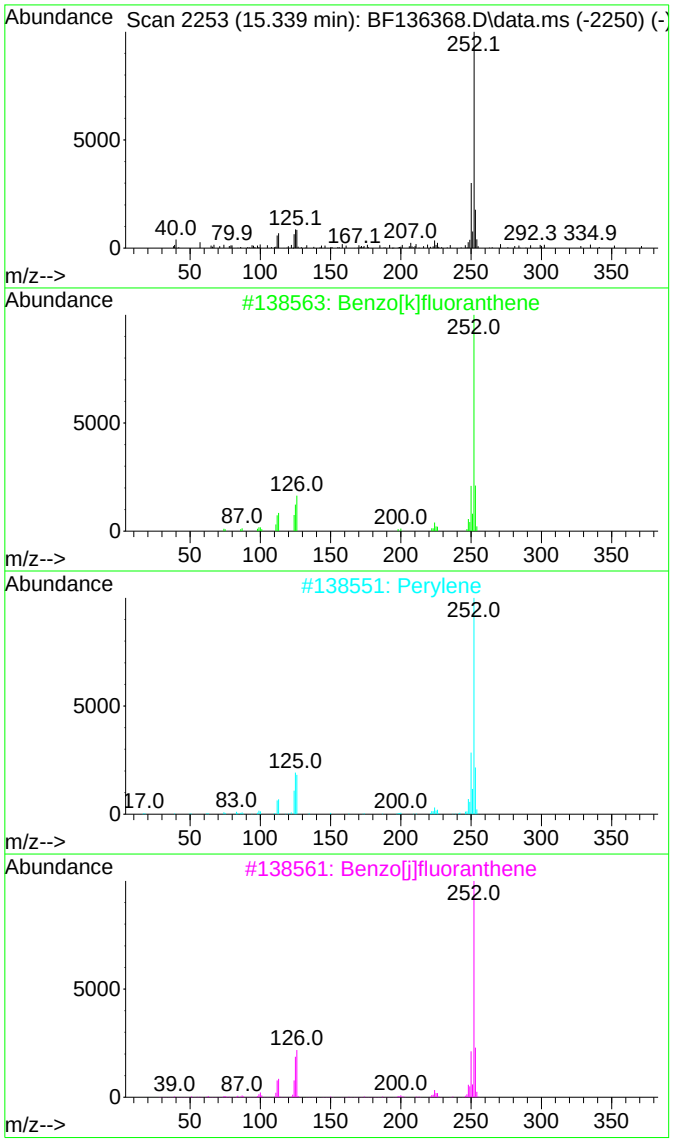
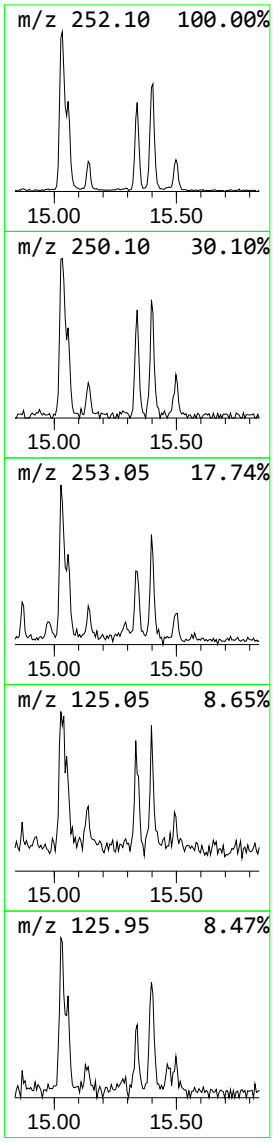
Peak Number 9 Perylene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.339	2.36 ng	55790	Perylene-d12	15.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89
2	Perylene	252	C20H12	000198-55-0	76
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	76
4	Benzo[a]pyrene	252	C20H12	000050-32-8	74
5	Benzo[e]pyrene	252	C20H12	000192-97-2	68





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Data File : BF136368.D
Acq On : 02 Dec 2023 08:54
Operator : CG\JU
Sample : 05420-01
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12018

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.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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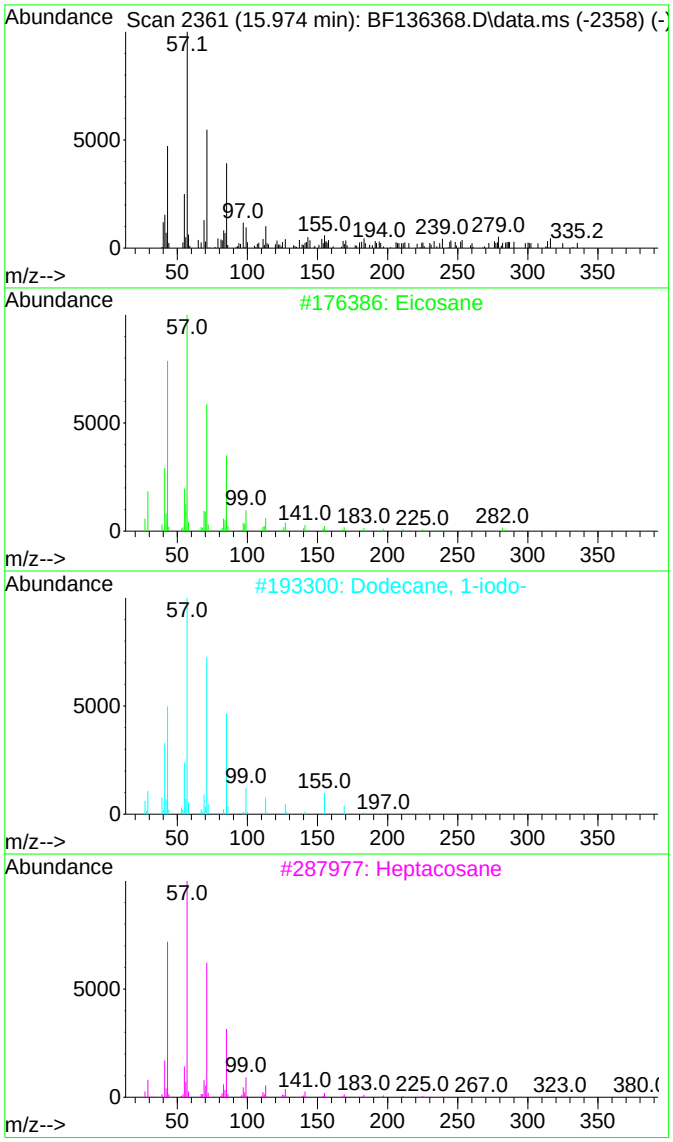
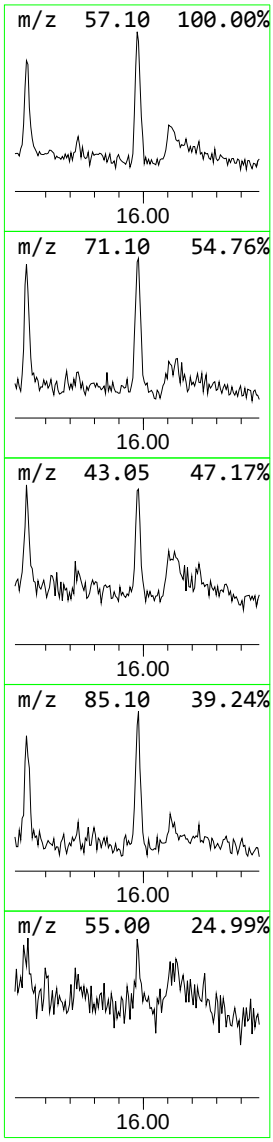
Peak Number 10 Dodecane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.974	2.46 ng	58193	Perylene-d12	15.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	81
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	72
3	Heptacosane	380	C27H56	000593-49-7	72
4	Hexatriacontane	507	C36H74	000630-06-8	72
5	Tridecane	184	C13H28	000629-50-5	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
Data File : BF136368.D
Acq On : 02 Dec 2023 08:54
Operator : CG\JU
Sample : 05420-01
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12018

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.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
unknown5.040	5.040	2.4	ng	72949	1	6.804	598132	20.0
(1S)-2,6,6-Trim...	6.093	16.7	ng	499249	1	6.804	598132	20.0
.beta.-Pinene	6.510	6.7	ng	199985	1	6.804	598132	20.0
n-Hexadecanoic ...	11.869	5.1	ng	151804	4	11.328	597548	20.0
n-Heptadecanol-1	12.433	26.9	ng	803483	4	11.328	597548	20.0
(1aR,4aS,8aS)-4...	14.210	2.2	ng	163507	5	13.986	1511910	20.0
Eicosane	15.127	2.5	ng	59509	6	15.469	473124	20.0
Perylene	15.339	2.4	ng	55790	6	15.469	473124	20.0
Dodecane, 1-iodo-	15.974	2.5	ng	58193	6	15.469	473124	20.0