LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139299.D
Acq On : 10 Sep 2024 14:58
Operator : RC/JU
Sample : P3905-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3A

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-BF090424.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139299.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	12	20	28	rVB	1389592	2151073	65.39%	8.151%
2	5.110	504	513	522	rVB	134116	215696	6.56%	0.817%
3	5.510	574	581	586	rBV	2015417	2803306	85.22%	10.623%
4	6.510	744	751	757	rBV	2037662	2945537	89.54%	11.162%
5	6.887	810	815	820	rVB	617912	738238	22.44%	2.798%
6	7.451	904	911	916	rBV	1395918	1910540	58.08%	7.240%
7	7.698	949	953	960	rVB	52582	63774	1.94%	0.242%
8	8.169	1024	1033	1038	rBV	779756	956308	29.07%	3.624%
9	9.245	1210	1216	1221	rBV	2634910	3289478	100.00%	12.465%
10	9.922	1326	1331	1336	rBV	811424	1012961	30.79%	3.839%
11	10.639	1447	1453	1459	rBV	491300	601100	18.27%	2.278%
12	10.710	1460	1465	1477	rBV	1370272	1771636	53.86%	6.714%
13	10.945	1501	1505	1511	rVB	46265	57830	1.76%	0.219%
14	11.410	1579	1584	1592	rBV2	735889	1041285	31.66%	3.946%
15	11.480	1592	1596	1600	rVB	35495	45536	1.38%	0.173%
16	11.933	1665	1673	1679	rBV2	157091	253103	7.69%	0.959%
17	12.022	1684	1688	1697	rVB	53606	100637	3.06%	0.381%
18	12.210	1713	1720	1727	rBV3	15752	37108	1.13%	0.141%
19	12.621	1785	1790	1795	rBV	336694	425384	12.93%	1.612%
20	12.721	1803	1807	1813	rBV3	21848	37539	1.14%	0.142%
21	12.851	1821	1829	1834	rBV	300962	439055	13.35%	1.664%
22	12.898	1834	1837	1843	rVB3	34601	49740	1.51%	0.188%
23	12.998	1845	1854	1859	rBV	1697200	2161353	65.71%	8.190%
24	13.069	1861	1866	1873	rBV3	28143	55122	1.68%	0.209%
25	13.174	1877	1884	1889	rVB	42320	87459	2.66%	0.331%
26	13.245	1889	1896	1899	rBV2	30300	53667	1.63%	0.203%
27	13.280	1899	1902	1910	rVB2	35562	51362	1.56%	0.195%
28	13.586	1945	1954	1959	rBV8	17751	55797	1.70%	0.211%
29	13.686	1966	1971	1976	rVB	24363	39221	1.19%	0.149%
30	13.798	1985	1990	1992	rBV2	25810	41574	1.26%	0.158%
31	13.892	2002	2006	2024	rVB5	71381	166939	5.07%	0.633%
32	14.045	2026	2032	2043	rVB2	534201	1013951	30.82%	3.842%
33	14.151	2046	2050	2054	rBV	24629	33917	1.03%	0.129%
34	14.433	2094	2098	2101	rBV	29561	37452	1.14%	0.142%
35	14.527	2109	2114	2117	rBV3	30529	52892	1.61%	0.200%
36	14.557	2117	2119	2127	rVB5	26756	56734	1.72%	0.215%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139299.D
Acq On : 10 Sep 2024 14:58
Operator : RC/JU
Sample : P3905-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3A

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-BF090424.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.092	2204	2210	2221	rBV	171996	397233	12.08%	1.505%
38	15.198	2226	2228	2233	rVB	32276	40475	1.23%	0.153%
39	15.398	2257	2262	2268	rVB	85178	129903	3.95%	0.492%
40	15.462	2268	2273	2278	rVV	126537	192273	5.85%	0.729%
41	15.527	2278	2284	2296	rVB	337832	592456	18.01%	2.245%
42	16.998	2528	2534	2543	rVB2	48580	112644	3.42%	0.427%
43	17.445	2604	2610	2617	rBV	33293	69691	2.12%	0.264%

Sum of corrected areas: 26388979

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
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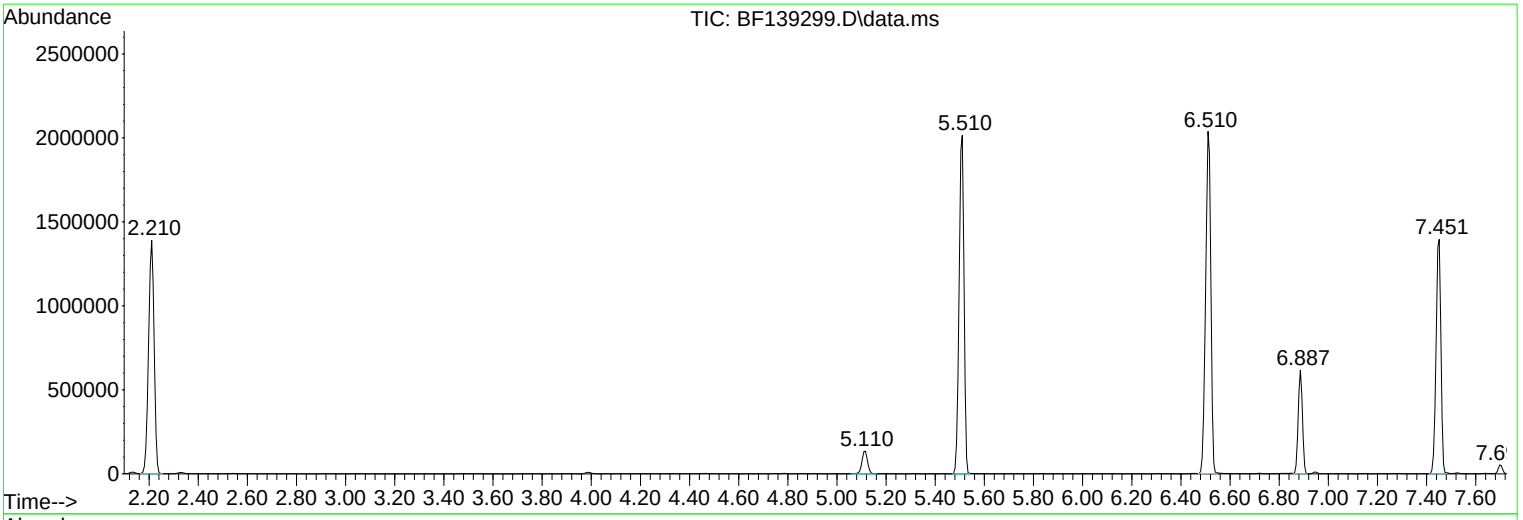
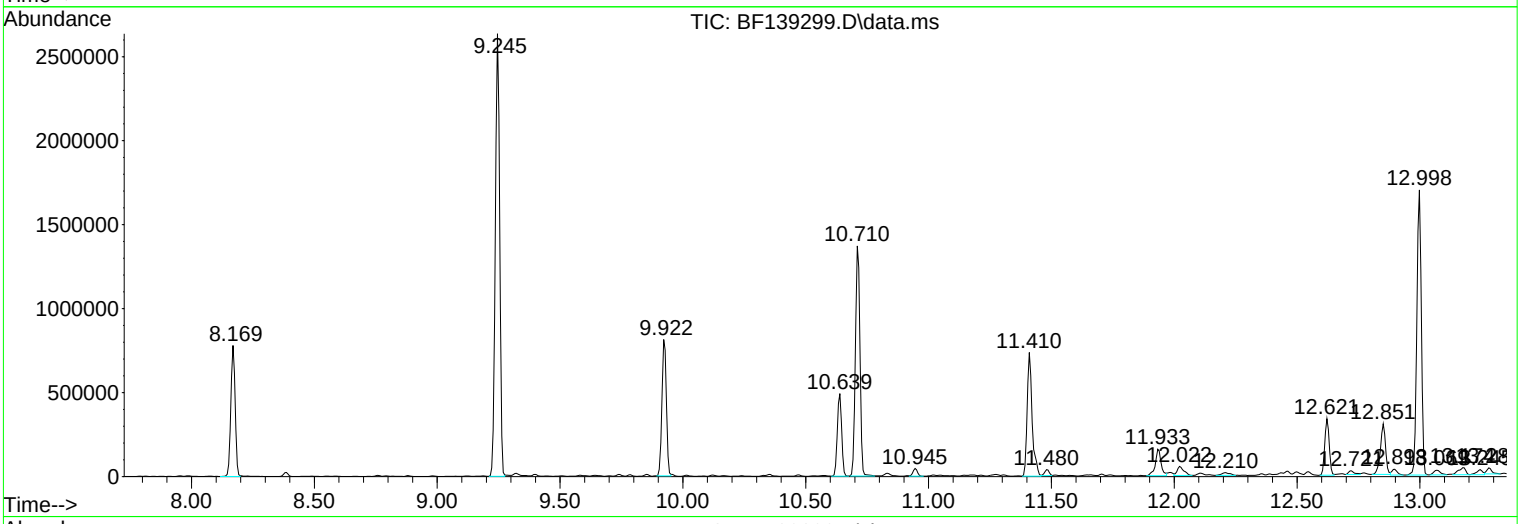
Misc :
ALS Vial : 8 Sample Multiplier: 1

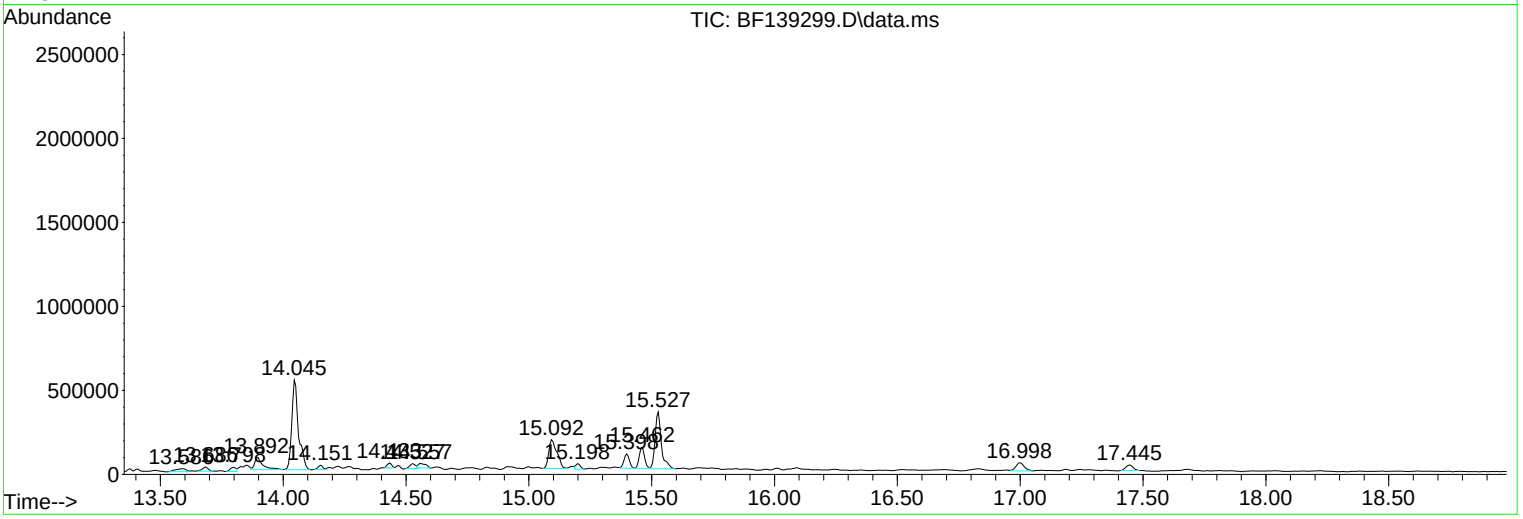
Instrument :
BNA_F
ClientSampleId :
TP-3A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139299.D
Acq On : 10 Sep 2024 14:58
Operator : RC/JU
Sample : P3905-01
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Instrument :
BNA_F
ClientSampleId :
TP-3A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

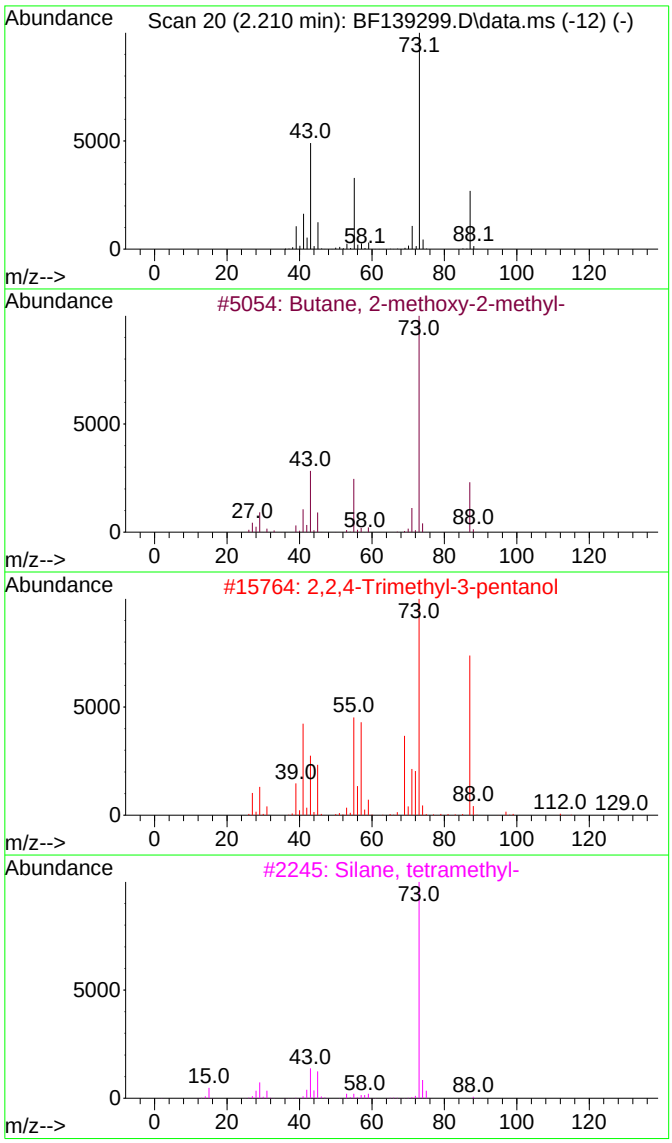
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

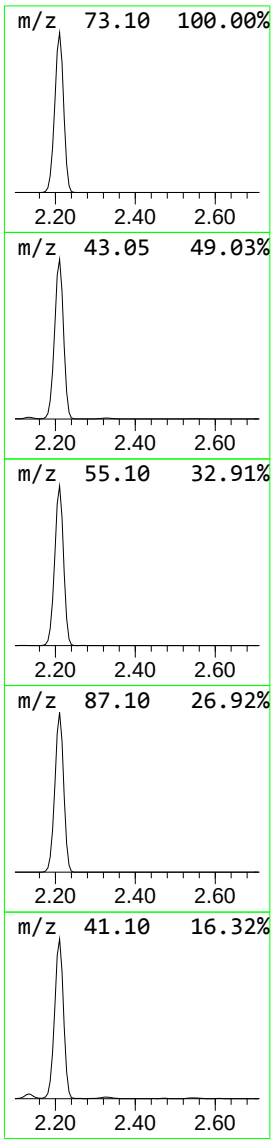
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.210	58.28 ng	2151070	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139299.D
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Operator : RC/JU
Sample : P3905-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3A

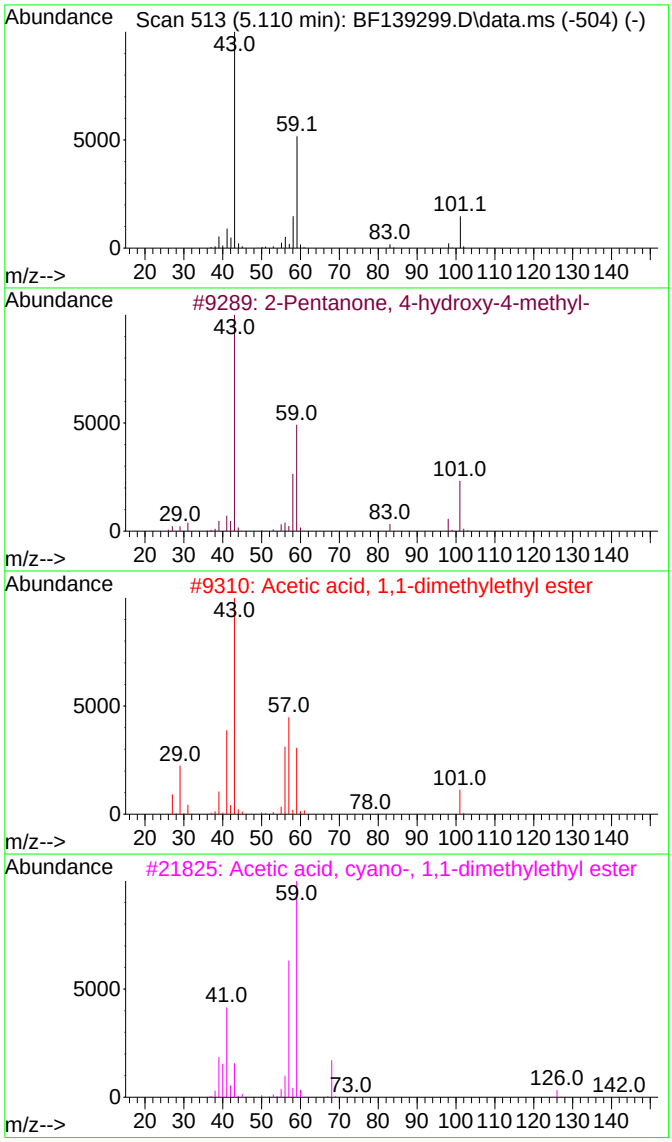
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

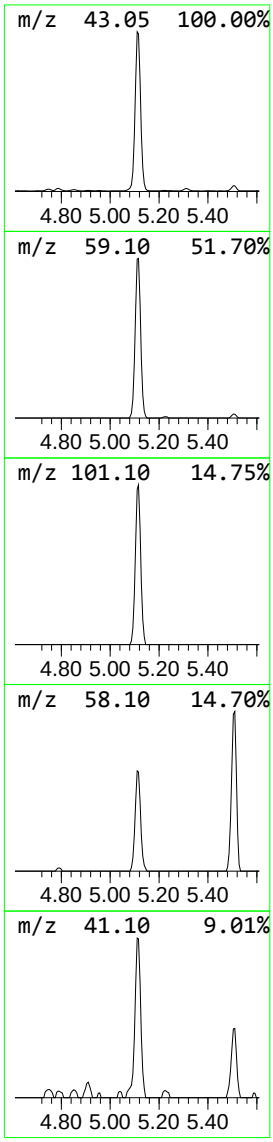
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	5.84 ng	215696	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139299.D
Acq On : 10 Sep 2024 14:58
Operator : RC/JU
Sample : P3905-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

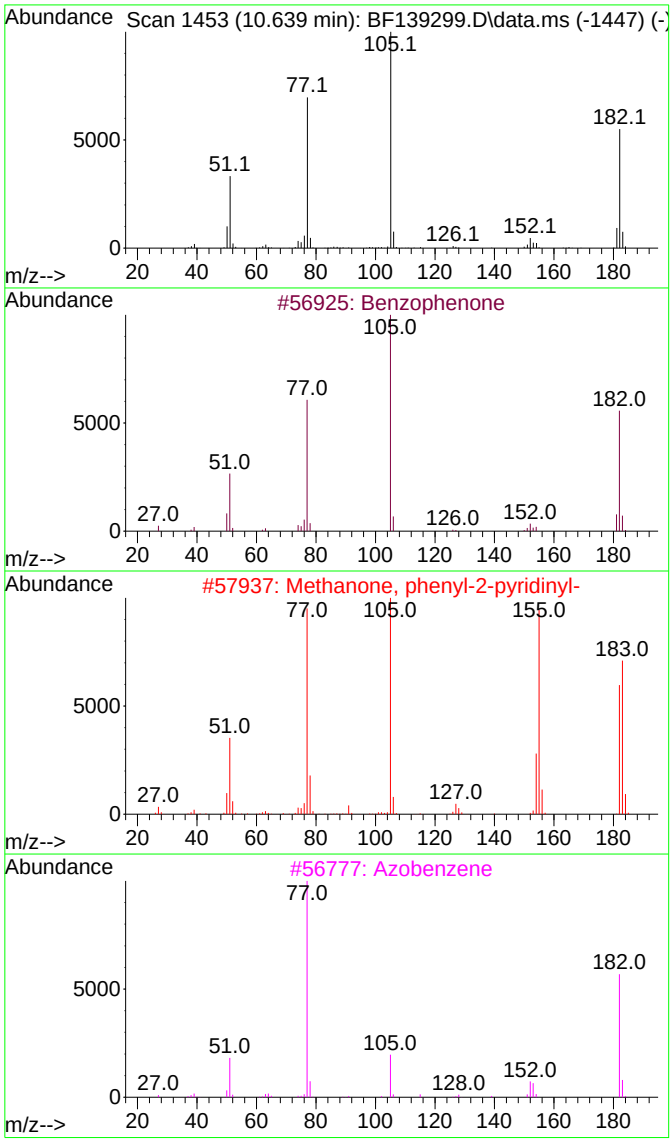
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

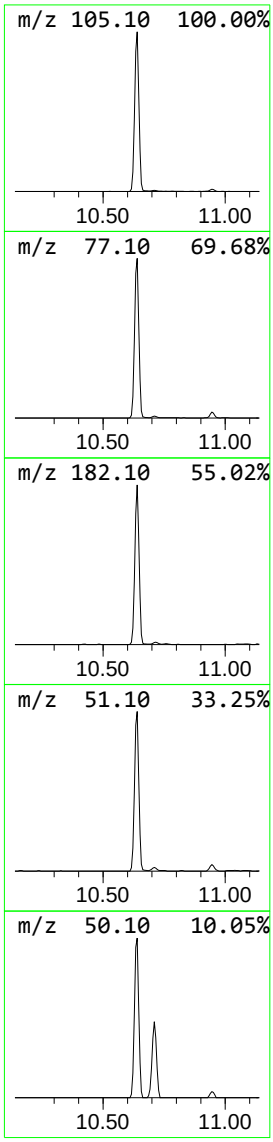
****

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.639	11.87 ng	601100	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	72
3	Azobenzene	182	C12H10N2	000103-33-3	52
4	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
5	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
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Sample : P3905-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

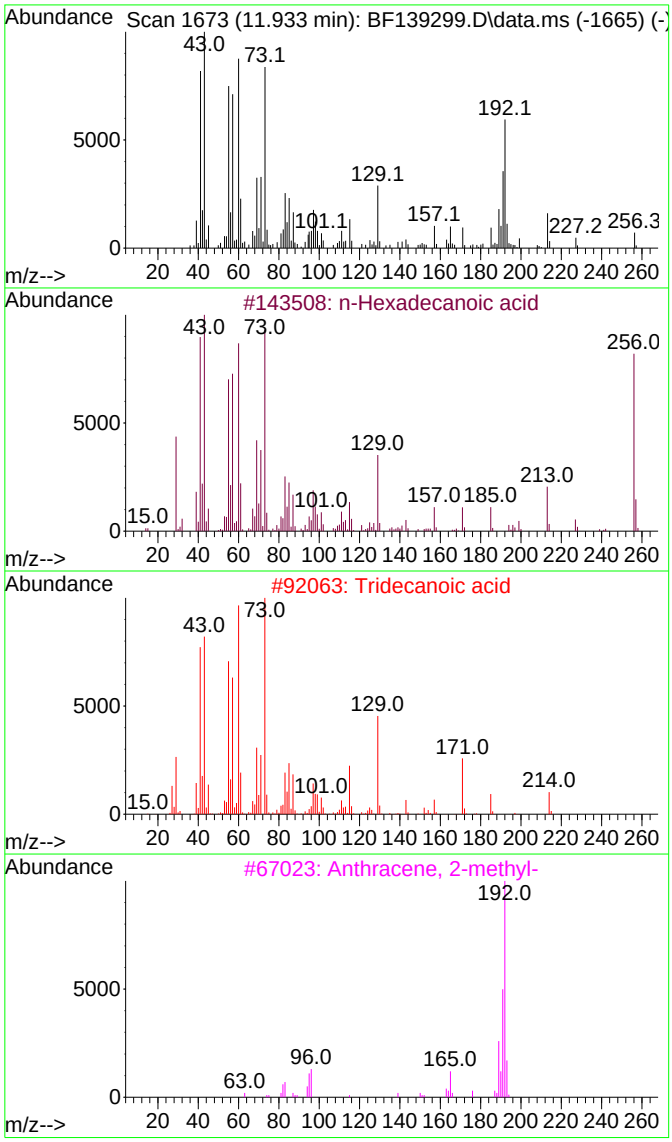
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

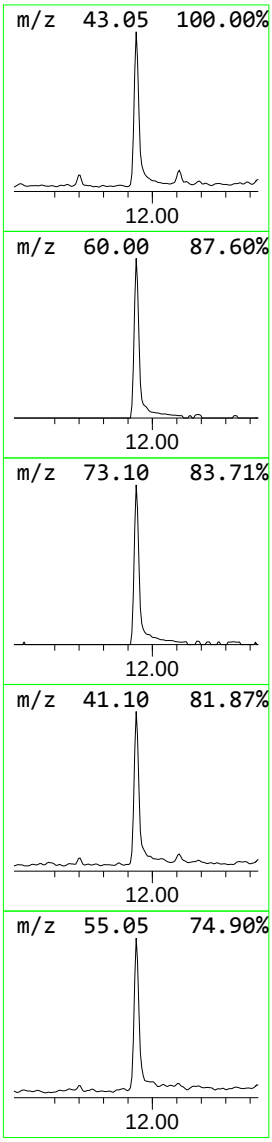
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	4.86 ng	253103	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	90
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	68
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	68





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Data File : BF139299.D
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Operator : RC/JU
Sample : P3905-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3A

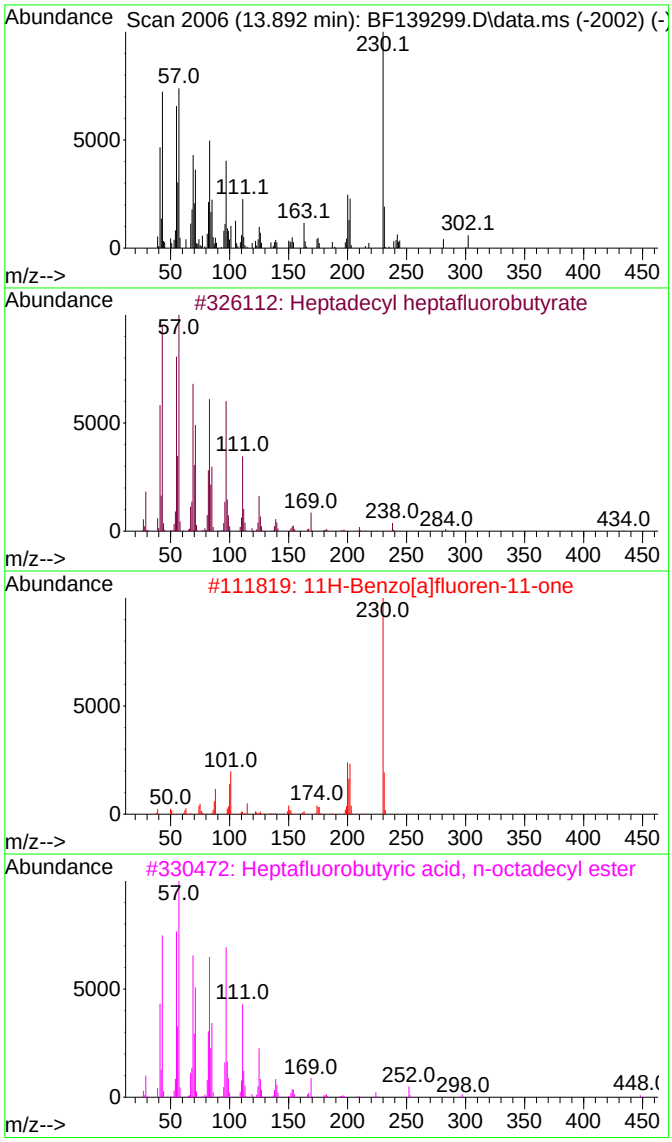
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

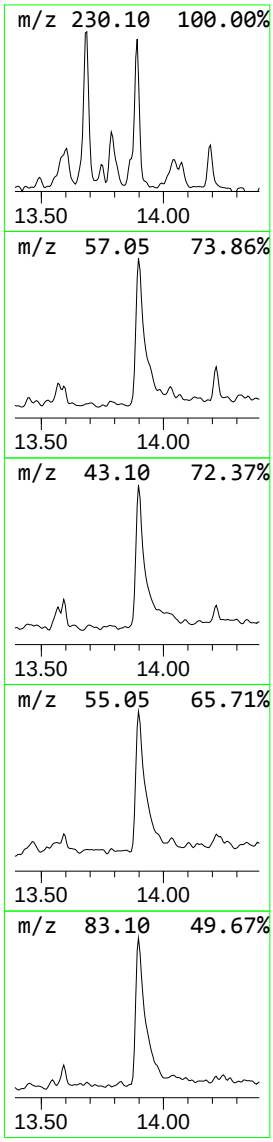
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	3.29 ng	166939	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	59
2	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	50
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	46
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	46
5	Triacontan-15-ol	438	C30H62O	031849-26-0	46





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ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

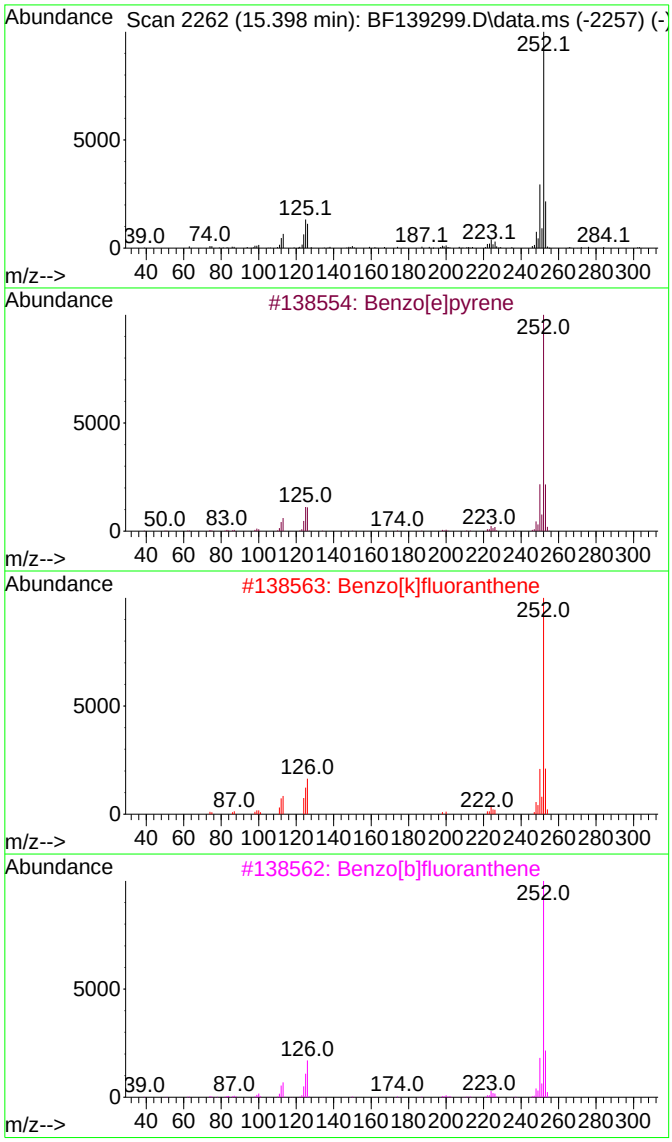
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

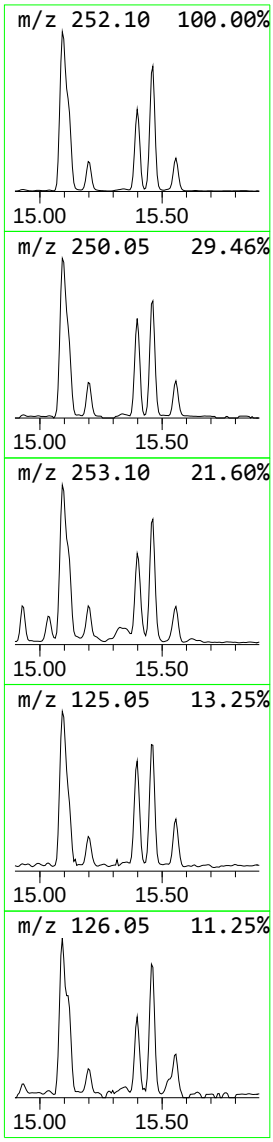
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.398	4.39 ng	129903	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	94
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	91
5	Perylene	252	C20H12	000198-55-0	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139299.D
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Operator : RC/JU
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.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
Butane, 2-metho...	2.210	58.3	ng	2151070	1	6.887	738238	20.0
2-Pentanone, 4-...	5.110	5.8	ng	215696	1	6.887	738238	20.0
Benzophenone	10.639	11.9	ng	601100	3	9.922	1012960	20.0
n-Hexadecanoic ...	11.933	4.9	ng	253103	4	11.410	1041290	20.0
Heptadecyl hept...	13.892	3.3	ng	166939	5	14.051	1013950	20.0
Benzo[e]pyrene	15.398	4.4	ng	129903	6	15.527	592456	20.0