LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080324\
Data File : BF138768.D
Acq On : 03 Aug 2024 14:09
Operator : RC/JU
Sample : P3448-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP4

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-BF073024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138768.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	9	21	rVB	792862	1246406	72.76%	8.315%
2	3.387	216	220	237	rBV	14664	40377	2.36%	0.269%
3	5.069	501	506	517	rVB	68354	106113	6.19%	0.708%
4	5.475	570	575	596	rBV	1035118	1408227	82.21%	9.395%
5	6.487	741	747	772	rVB	1104379	1497399	87.41%	9.990%
6	6.675	772	779	792	rBV3	11644	22628	1.32%	0.151%
7	6.845	803	808	813	rBV	325427	398242	23.25%	2.657%
8	7.410	897	904	909	rBV	699842	928023	54.17%	6.191%
9	8.122	1017	1025	1033	rBV	396452	531760	31.04%	3.548%
10	8.439	1074	1079	1092	rBV	44624	71628	4.18%	0.478%
11	9.198	1202	1208	1213	rBV	1368033	1713043	100.00%	11.429%
12	9.880	1315	1324	1328	rBV	460314	594381	34.70%	3.965%
13	9.910	1328	1329	1334	rVV	29298	24175	1.41%	0.161%
14	9.975	1334	1340	1346	rVB2	42421	67456	3.94%	0.450%
15	10.427	1412	1417	1421	rBV3	22924	30393	1.77%	0.203%
16	10.669	1453	1458	1469	rBV	807386	1066536	62.26%	7.115%
17	10.780	1473	1477	1485	rVB6	14915	29718	1.73%	0.198%
18	11.221	1547	1552	1555	rBV3	15282	22758	1.33%	0.152%
19	11.369	1571	1577	1580	rBV	421454	646118	37.72%	4.311%
20	11.439	1585	1589	1593	rVB	36167	46933	2.74%	0.313%
21	11.869	1657	1662	1663	rBV	42764	49568	2.89%	0.331%
22	11.892	1663	1666	1671	rVV2	96525	139030	8.12%	0.928%
23	11.945	1671	1675	1677	rVV	20944	32065	1.87%	0.214%
24	11.980	1677	1681	1690	rVB2	67633	140101	8.18%	0.935%
25	12.163	1708	1712	1715	rBV	30810	38502	2.25%	0.257%
26	12.192	1715	1717	1722	rVB	16492	19004	1.11%	0.127%
27	12.310	1733	1737	1740	rBV2	17089	23461	1.37%	0.157%
28	12.416	1751	1755	1758	rBV	31599	46123	2.69%	0.308%
29	12.451	1758	1761	1767	rVV3	26600	48339	2.82%	0.322%
30	12.504	1767	1770	1775	rVB2	18839	27809	1.62%	0.186%
31	12.580	1778	1783	1788	rBV	255159	318065	18.57%	2.122%
32	12.810	1815	1822	1829	rBV	264778	388277	22.67%	2.590%
33	12.951	1840	1846	1852	rVB	1104503	1407670	82.17%	9.391%
34	13.027	1854	1859	1865	rBV3	25876	47669	2.78%	0.318%
35	13.133	1870	1877	1881	rVB	31573	61206	3.57%	0.408%
36	13.204	1886	1889	1892	rVV	19363	24286	1.42%	0.162%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080324\
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Acq On : 03 Aug 2024 14:09
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Sample : P3448-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP4

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-BF073024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.239	1892	1895	1903	rVB2	29552	42665	2.49%	0.285%
38	13.333	1908	1911	1913	rVV	16045	18856	1.10%	0.126%
39	13.363	1913	1916	1924	rVB3	18402	35347	2.06%	0.236%
40	13.857	1995	2000	2009	rVB2	48678	89652	5.23%	0.598%
41	14.004	2019	2025	2038	rVB2	276498	524688	30.63%	3.500%
42	14.392	2087	2091	2095	rBV	22508	31441	1.84%	0.210%
43	15.045	2197	2202	2210	rBV	83028	181193	10.58%	1.209%
44	15.157	2217	2221	2226	rBV	16101	24656	1.44%	0.164%
45	15.351	2249	2254	2259	rVB	49147	76215	4.45%	0.508%
46	15.409	2259	2264	2269	rBV	72284	106574	6.22%	0.711%
47	15.474	2269	2275	2287	rBV	229661	391532	22.86%	2.612%
48	16.945	2519	2525	2532	rBV2	41601	86769	5.07%	0.579%
49	17.386	2595	2600	2616	rVB	33451	75893	4.43%	0.506%

Sum of corrected areas: 14988970

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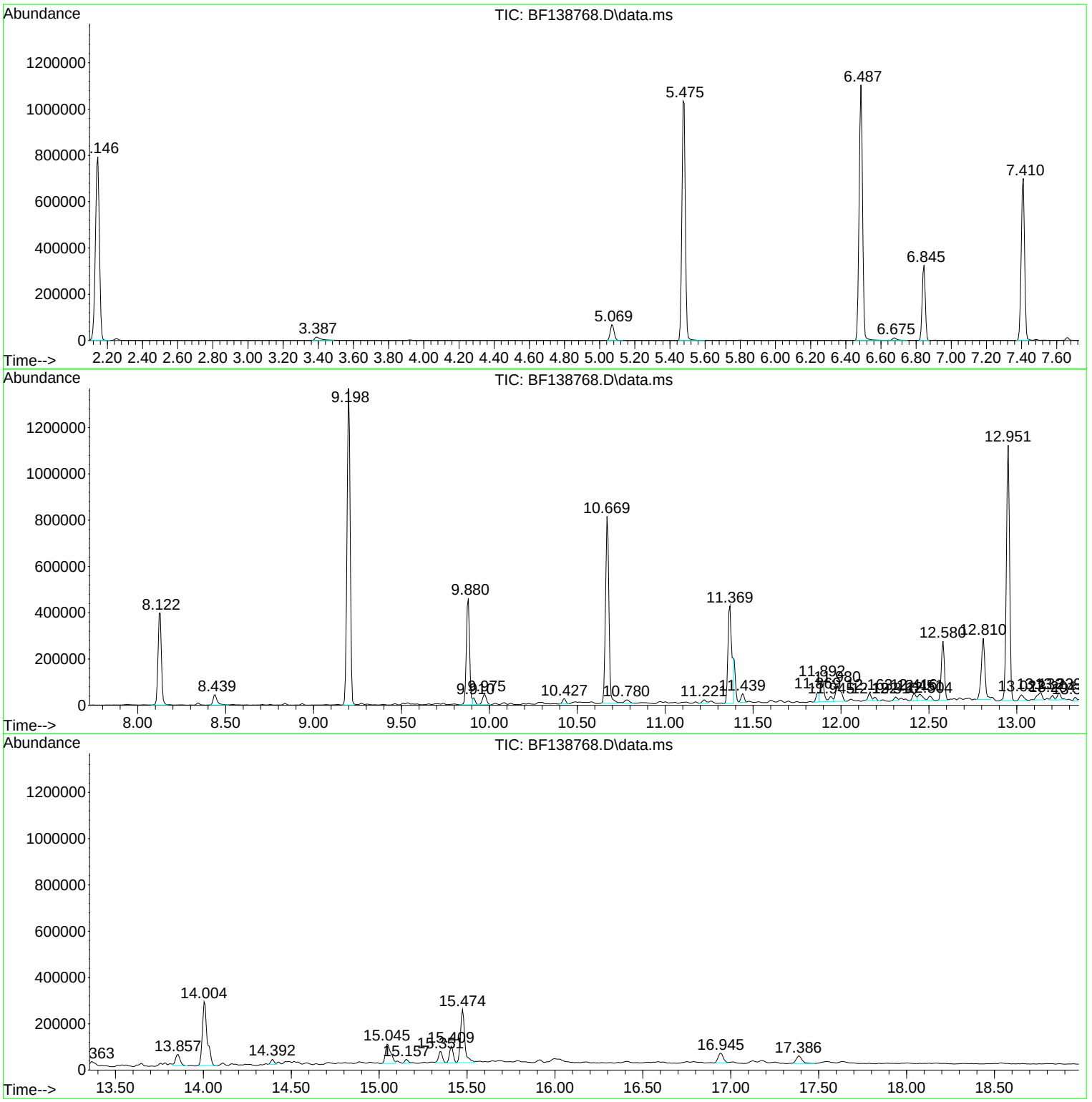
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080324\
Data File : BF138768.D
Acq On : 03 Aug 2024 14:09
Operator : RC/JU
Sample : P3448-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

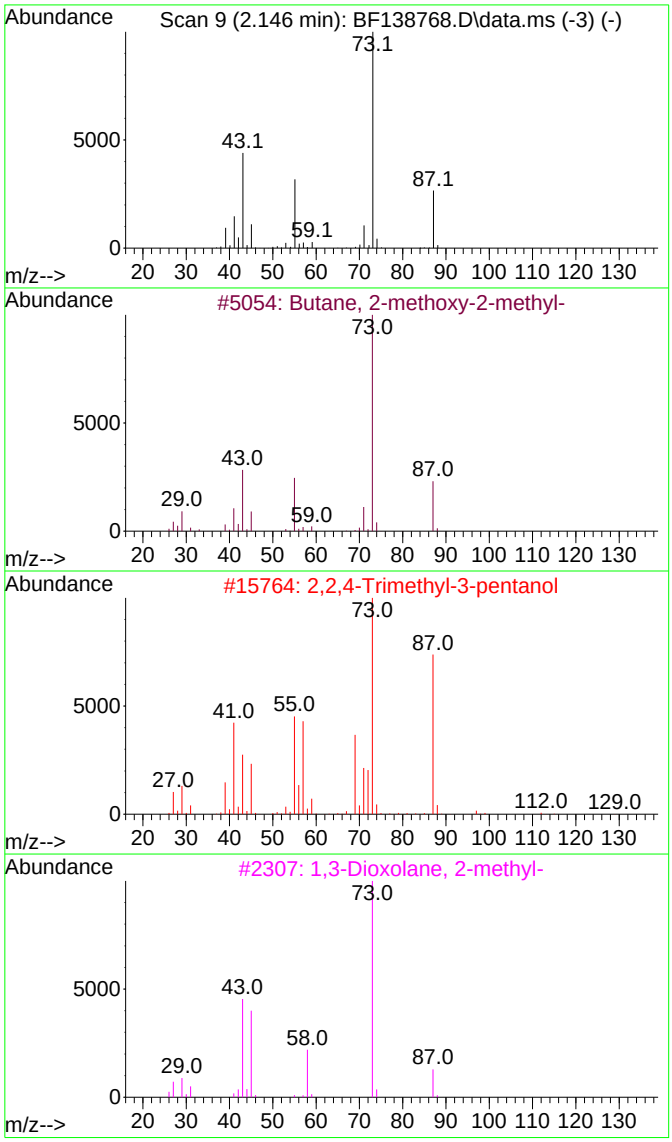
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

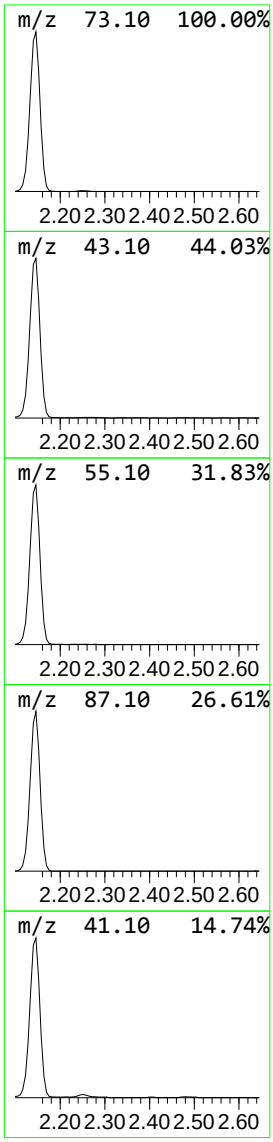
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	62.60 ng	1246410	1,4-Dichlorobenzene-d4	6.845

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080324\
Data File : BF138768.D
Acq On : 03 Aug 2024 14:09
Operator : RC/JU
Sample : P3448-07
Misc :
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

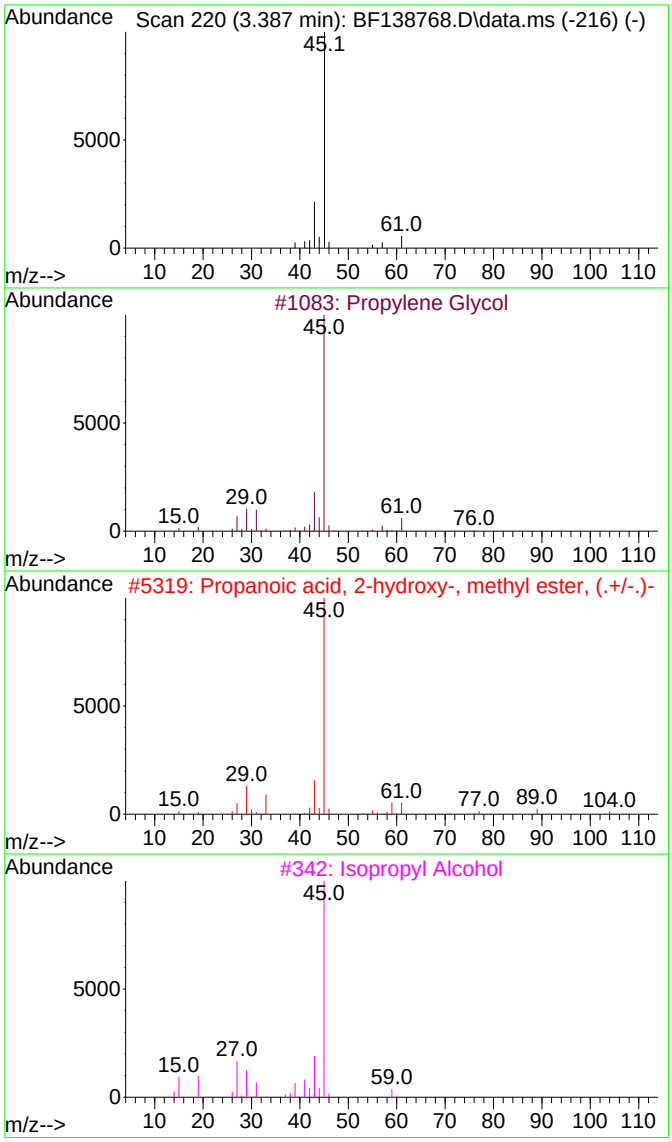
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

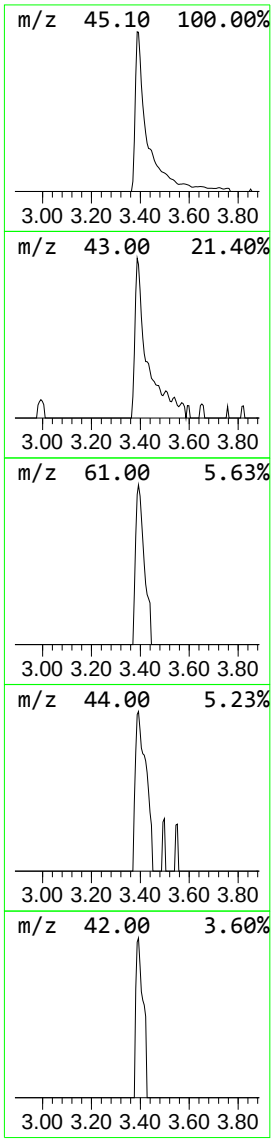
****

Peak Number 2 unknown3.387 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.387	2.03 ng	40377	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	9
2	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5	Formamide	45	CH3NO	000075-12-7	5





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Sample : P3448-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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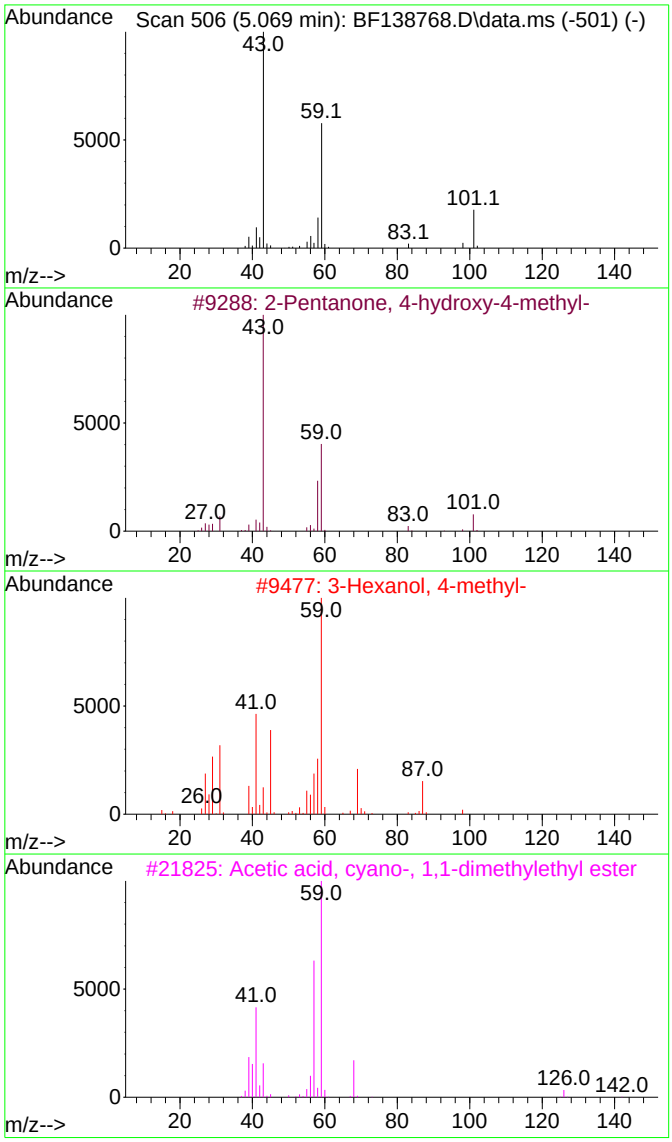
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

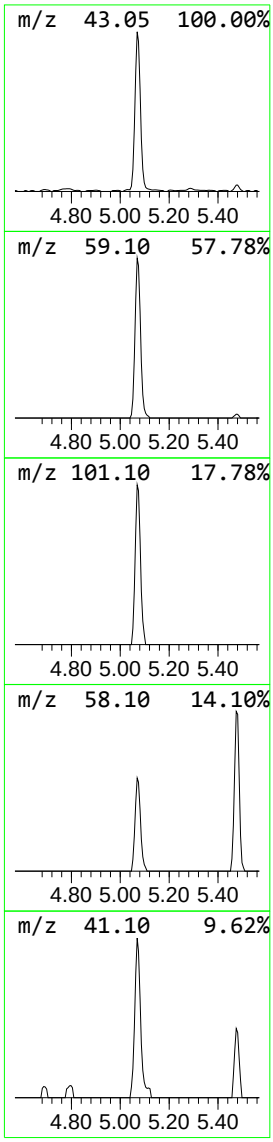
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	5.33 ng	106113	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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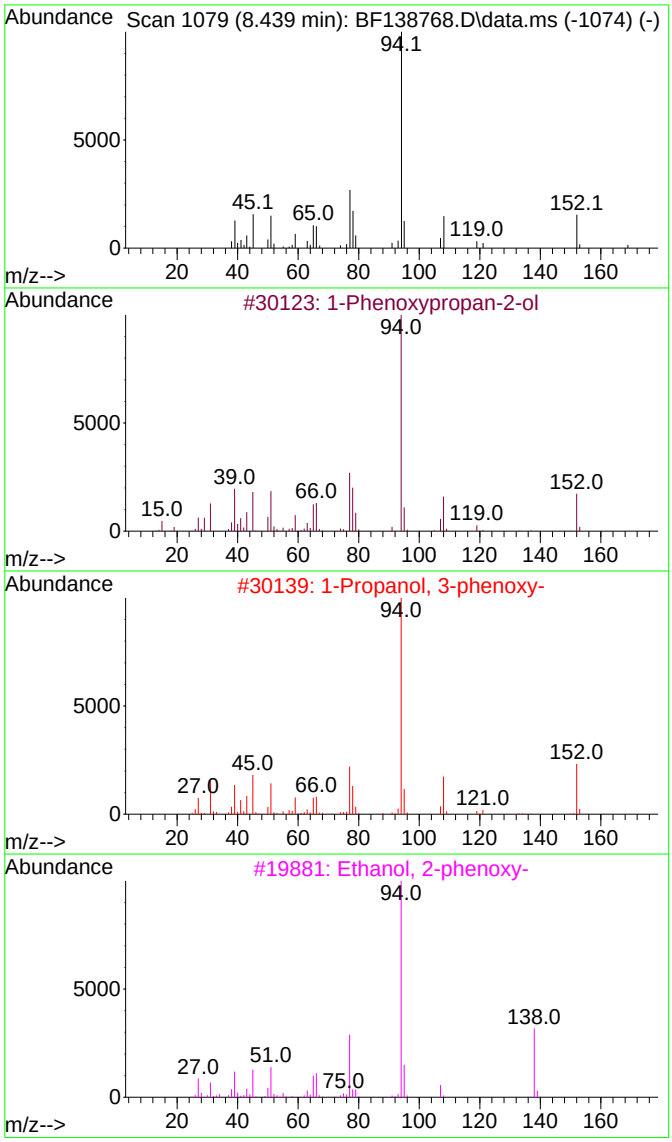
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

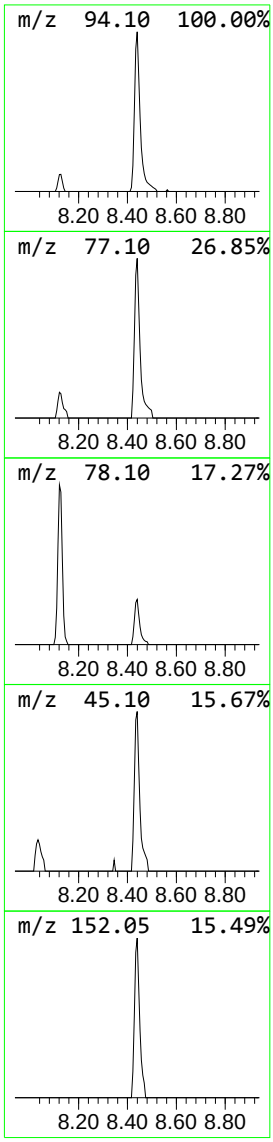
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.439	2.69 ng	71628	Naphthalene-d8	8.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
5	Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	53





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Sample : P3448-07
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

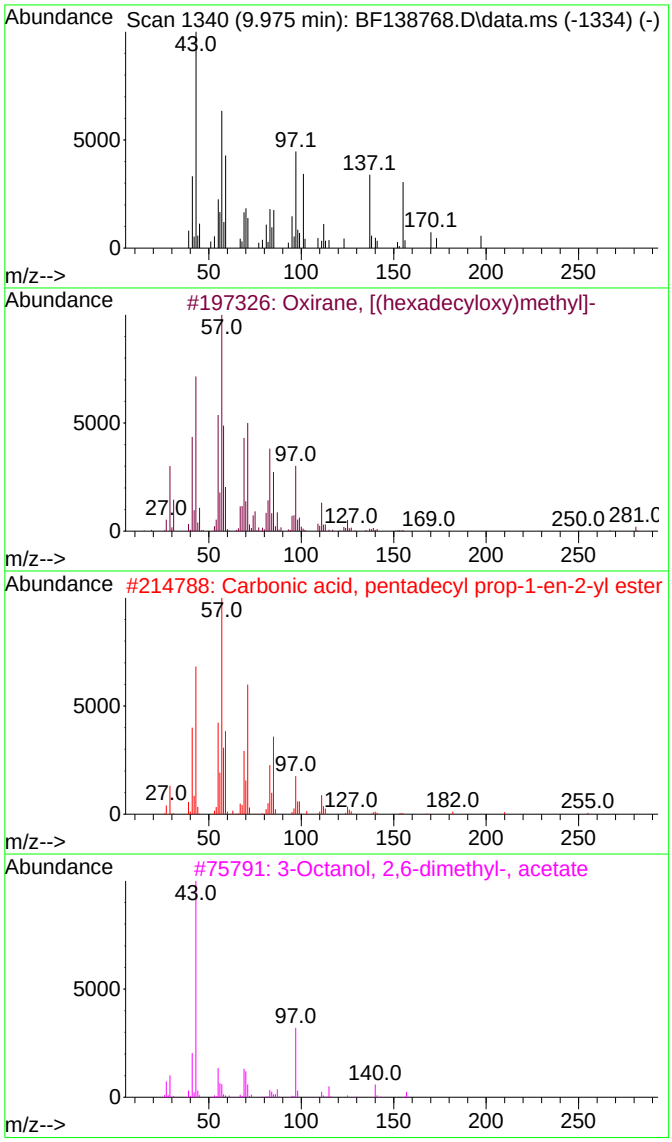
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

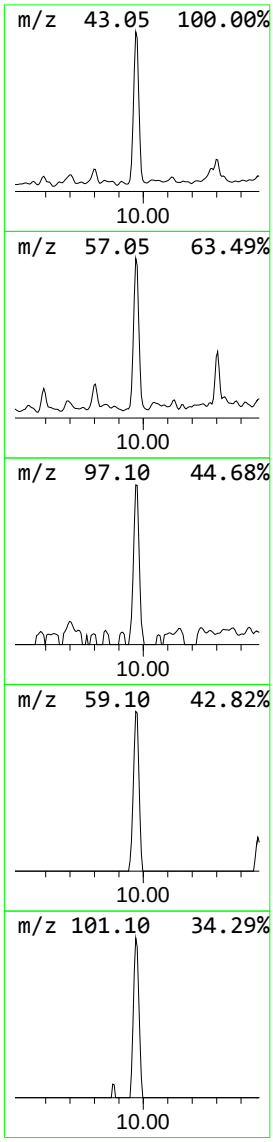
****

Peak Number 5 unknown9.975 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.975	2.27 ng	67456	Acenaphthene-d10	9.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(hexadecyloxy)methyl]-	298	C19H38O2	015965-99-8	12
2	Carbonic acid, pentadecyl prop-1...	312	C19H36O3	1000382-91-0	10
3	3-Octanol, 2,6-dimethyl-, acetate	200	C12H24O2	123232-57-5	10
4	Methyl 3,4,6-tri-O-acetyl-2-acet...	361	C15H23NO9	002595-39-3	10
5	5-Ethyl-3-nonanol	172	C11H24O	019780-71-3	10





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

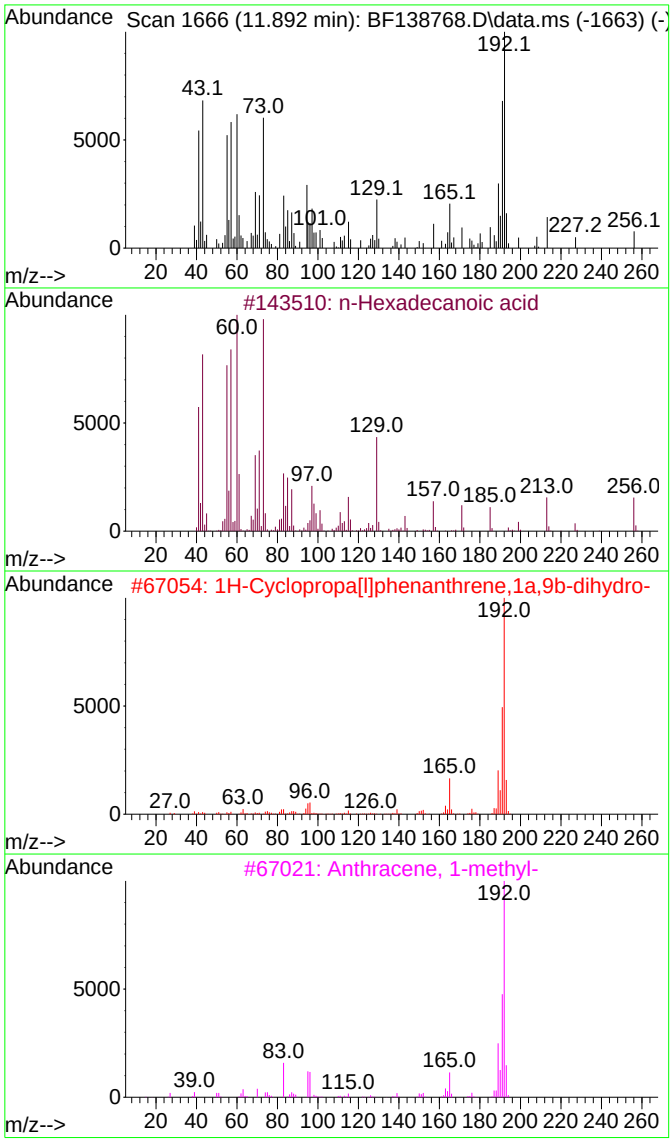
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

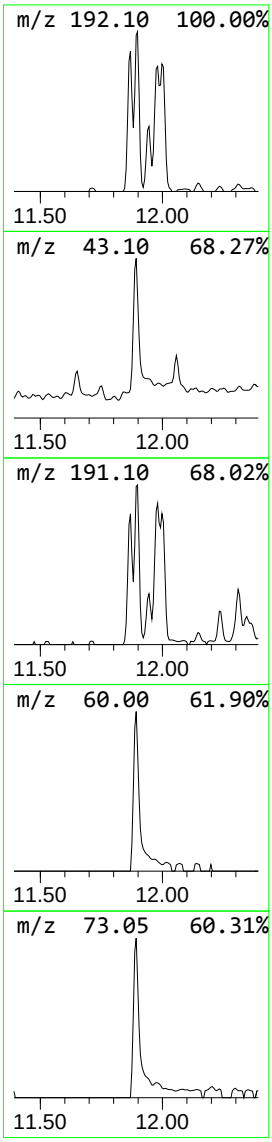
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	4.30 ng	139030	Phenanthrene-d10	11.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	70
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	64
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	64
5	Benzene, 1,1'-(1,2-propadienylid...	192	C15H12	014251-57-1	60





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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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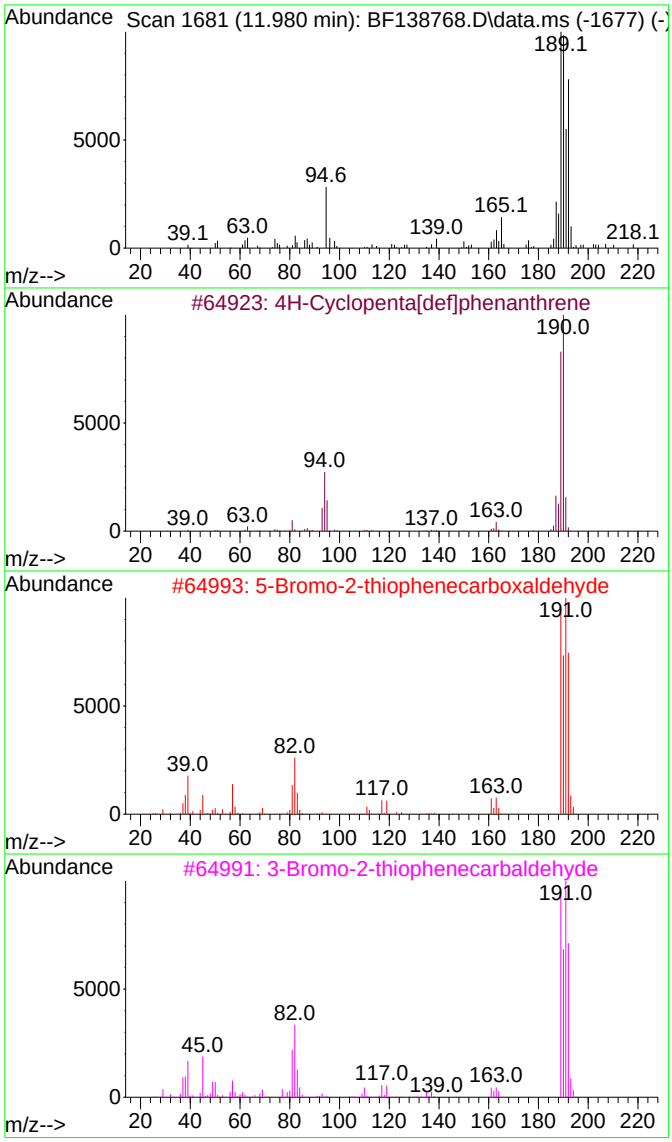
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

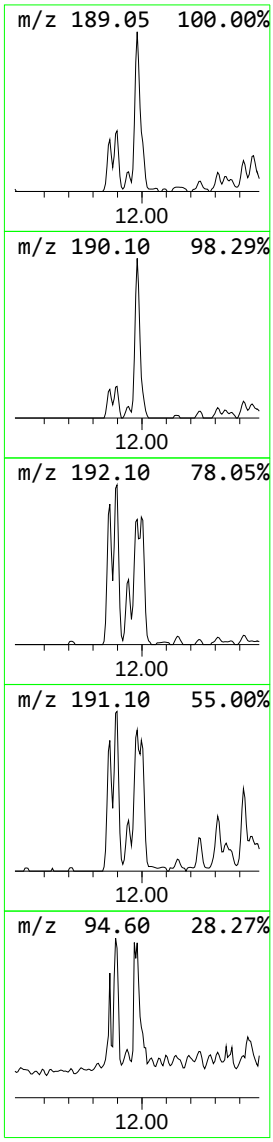
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.980	4.34 ng	140101	Phenanthrene-d10	11.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
2	5-Bromo-2-thiophenecarboxaldehyde	190	C5H3BrOS	004701-17-1	53
3	3-Bromo-2-thiophenecarbaldehyde	190	C5H3BrOS	000930-96-1	53
4	Benzene, 1,1'-(1,2-propadienylid...	192	C15H12	014251-57-1	38
5	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080324\
Data File : BF138768.D
Acq On : 03 Aug 2024 14:09
Operator : RC/JU
Sample : P3448-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

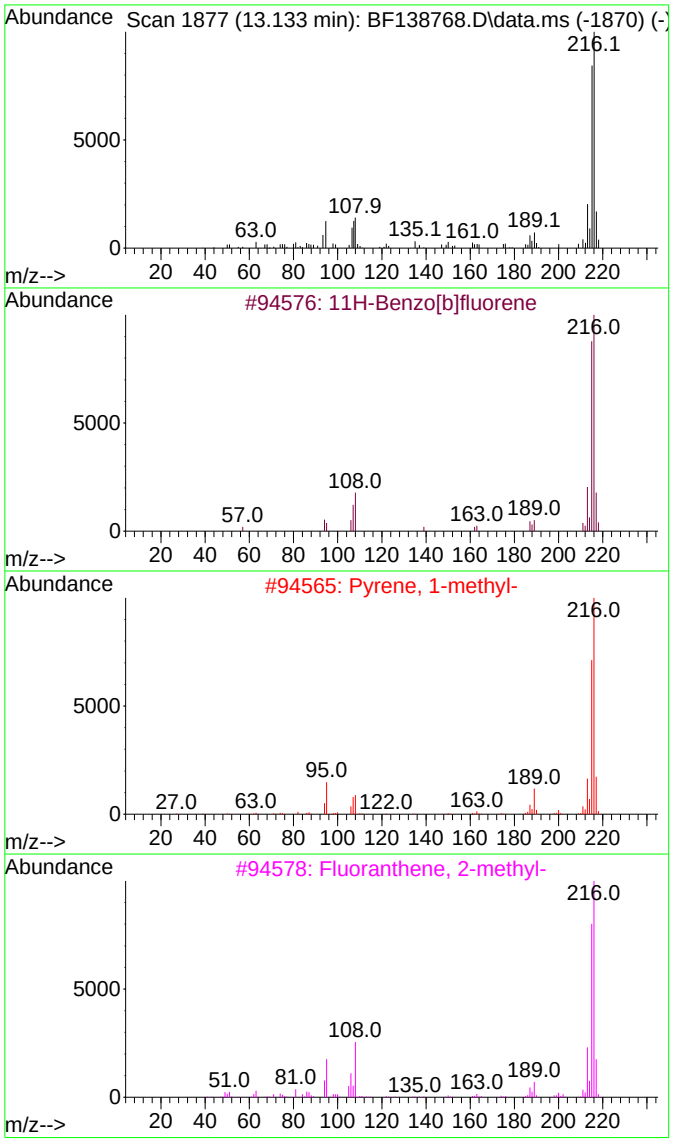
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

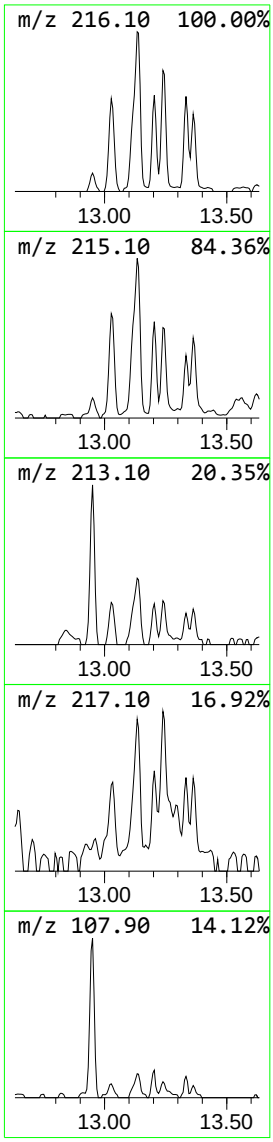
****

Peak Number 8 11H-Benzo[b]fluorene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.133	2.33 ng	61206	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	96
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
4	Pyrene, 2-methyl-	216	C17H12	003442-78-2	91
5	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87





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Acq On : 03 Aug 2024 14:09
Operator : RC/JU
Sample : P3448-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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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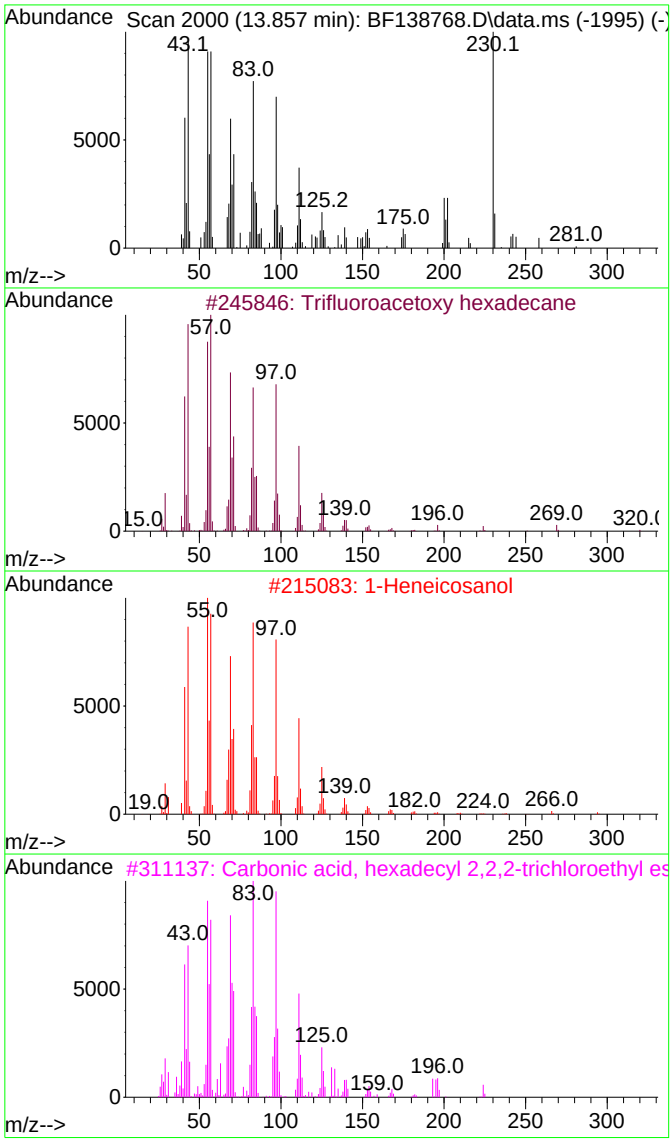
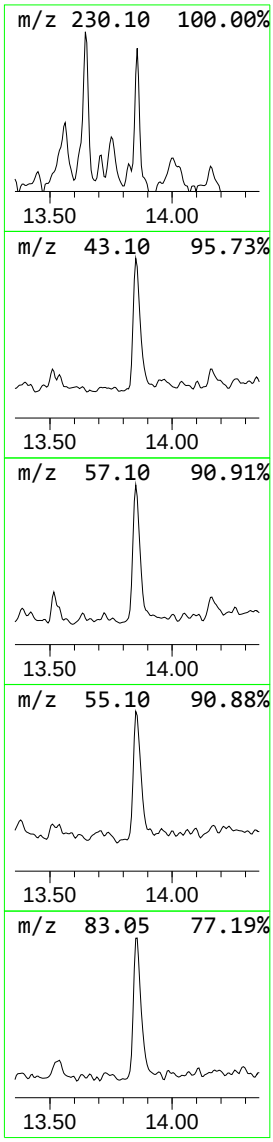
Peak Number 9 Trifluoroacetoxy hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	3.42 ng	89652	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
2	1-Heneicosanol	312	C21H44O	015594-90-8	87
3	Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	78
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	78
5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080324\
Data File : BF138768.D
Acq On : 03 Aug 2024 14:09
Operator : RC/JU
Sample : P3448-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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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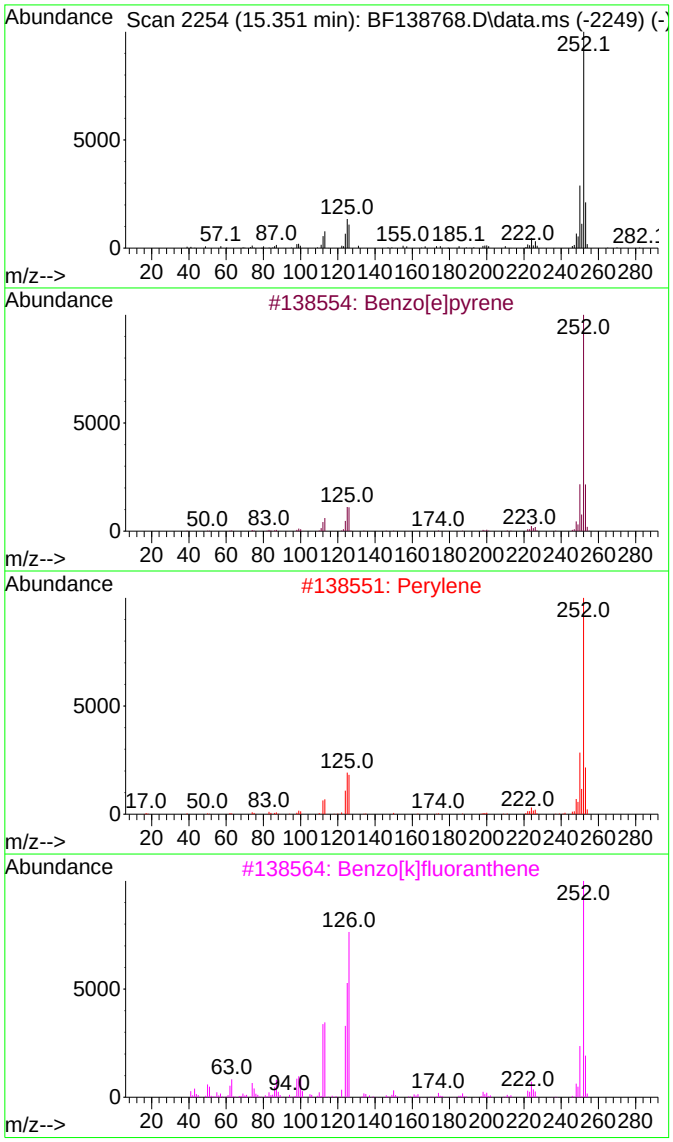
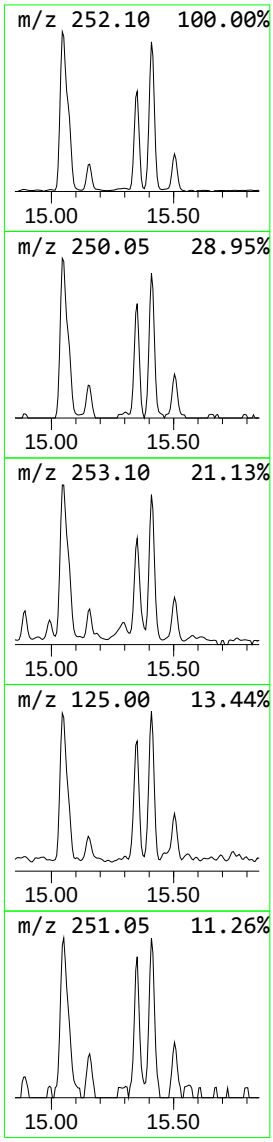
Peak Number 10 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.351	3.89 ng	76215	Perylene-d12	15.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Perylene	252	C20H12	000198-55-0	95
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080324\
Data File : BF138768.D
Acq On : 03 Aug 2024 14:09
Operator : RC/JU
Sample : P3448-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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...	2.146	62.6	ng	1246410	1	6.845	398242	20.0
unknown3.387	3.387	2.0	ng	40377	1	6.845	398242	20.0
2-Pentanone, 4-...	5.069	5.3	ng	106113	1	6.845	398242	20.0
1-Phenoxypropan...	8.439	2.7	ng	71628	2	8.128	531760	20.0
unknown9.975	9.975	2.3	ng	67456	3	9.880	594381	20.0
n-Hexadecanoic ...	11.892	4.3	ng	139030	4	11.368	646118	20.0
4H-Cyclopenta[d...	11.980	4.3	ng	140101	4	11.368	646118	20.0
11H-Benzo[b]flu...	13.133	2.3	ng	61206	5	14.010	524688	20.0
Trifluoroacetox...	13.857	3.4	ng	89652	5	14.010	524688	20.0
Benzo[e]pyrene	15.351	3.9	ng	76215	6	15.474	391532	20.0