LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
Data File : BF138658.D
Acq On : 25 Jul 2024 17:50
Operator : RC/JU
Sample : P3357-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-857-J-SO-1-1.5-072024

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-BF070924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138658.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	7	20	rVB	804897	1214708	75.20%	7.526%
2	3.363	211	216	240	rBV	39256	102744	6.36%	0.637%
3	5.069	495	506	513	rVB	74036	108278	6.70%	0.671%
4	5.475	570	575	586	rBV	1085272	1459865	90.38%	9.045%
5	6.487	741	747	764	rBV	1158684	1523635	94.33%	9.441%
6	6.681	775	780	792	rVB	29114	40776	2.52%	0.253%
7	6.851	804	809	814	rBV	403353	485307	30.05%	3.007%
8	7.416	898	905	910	rBV	745996	975273	60.38%	6.043%
9	7.669	943	948	954	rVB	12323	16205	1.00%	0.100%
10	8.134	1021	1027	1035	rBV	520481	657943	40.73%	4.077%
11	8.445	1075	1080	1095	rBV	74912	110735	6.86%	0.686%
12	9.204	1204	1209	1220	rBV	1253347	1615237	100.00%	10.008%
13	9.886	1319	1325	1329	rBV	566187	716613	44.37%	4.440%
14	9.916	1329	1330	1335	rVV	48151	41906	2.59%	0.260%
15	9.975	1335	1340	1348	rVB	50826	79799	4.94%	0.494%
16	10.092	1356	1360	1364	rBV	17077	21326	1.32%	0.132%
17	10.433	1413	1418	1422	rBV	35315	41755	2.59%	0.259%
18	10.675	1453	1459	1474	rBV	707979	938800	58.12%	5.817%
19	11.228	1548	1553	1556	rVV4	10464	16230	1.00%	0.101%
20	11.269	1556	1560	1564	rVB	18568	23381	1.45%	0.145%
21	11.369	1572	1577	1580	rBV	502361	748116	46.32%	4.635%
22	11.392	1580	1581	1586	rVV	387146	355896	22.03%	2.205%
23	11.445	1586	1590	1594	rVB	68223	82928	5.13%	0.514%
24	11.604	1610	1617	1623	rBV2	36799	55088	3.41%	0.341%
25	11.757	1638	1643	1650	rBV2	14751	20039	1.24%	0.124%
26	11.869	1658	1662	1664	rBV	25252	32946	2.04%	0.204%
27	11.898	1664	1667	1671	rVB2	44951	56677	3.51%	0.351%
28	11.986	1678	1682	1690	rVB2	51087	86800	5.37%	0.538%
29	12.163	1708	1712	1715	rBV	18769	25767	1.60%	0.160%
30	12.192	1715	1717	1722	rVB	25005	27666	1.71%	0.171%
31	12.457	1759	1762	1767	rVV2	11616	17668	1.09%	0.109%
32	12.580	1778	1783	1789	rBV	394989	493218	30.54%	3.056%
33	12.810	1815	1822	1828	rVV	305425	453527	28.08%	2.810%
34	12.951	1838	1846	1853	rVB	807265	1023843	63.39%	6.344%
35	13.027	1853	1859	1863	rBV2	15679	29592	1.83%	0.183%
36	13.139	1869	1878	1882	rBV2	30910	57828	3.58%	0.358%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
Data File : BF138658.D
Acq On : 25 Jul 2024 17:50
Operator : RC/JU
Sample : P3357-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-857-J-SO-1-1.5-072024

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-BF070924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.204	1886	1889	1892	rBV2	25009	26831	1.66%	0.166%
38	13.239	1892	1895	1898	rBV2	15052	17863	1.11%	0.111%
39	13.645	1957	1964	1969	rBV2	17379	29643	1.84%	0.184%
40	13.757	1978	1983	1985	rBV2	24253	33621	2.08%	0.208%
41	13.851	1995	1999	2008	rVB2	60759	102389	6.34%	0.634%
42	14.004	2016	2025	2029	rBV2	395616	685870	42.46%	4.250%
43	14.110	2038	2043	2047	rBV	26661	34827	2.16%	0.216%
44	14.233	2061	2064	2067	rVB2	14814	19333	1.20%	0.120%
45	14.392	2087	2091	2094	rVB2	16233	20055	1.24%	0.124%
46	14.486	2101	2107	2110	rBV5	21996	48211	2.98%	0.299%
47	14.704	2137	2144	2150	rBV7	11419	30189	1.87%	0.187%
48	14.757	2150	2153	2160	rVB6	9108	22162	1.37%	0.137%
49	15.045	2196	2202	2210	rBV	142983	314986	19.50%	1.952%
50	15.110	2210	2213	2216	rVV2	20817	26378	1.63%	0.163%
51	15.151	2216	2220	2224	rVV	19075	24591	1.52%	0.152%
52	15.257	2232	2238	2240	rBV4	7362	16874	1.04%	0.105%
53	15.345	2248	2253	2259	rVB	75627	117943	7.30%	0.731%
54	15.410	2259	2264	2269	rVB	101977	152422	9.44%	0.944%
55	15.468	2269	2274	2287	rVB	264814	450925	27.92%	2.794%
56	15.686	2308	2311	2318	rVB5	15427	24932	1.54%	0.154%
57	15.915	2344	2350	2358	rBV2	21497	42986	2.66%	0.266%
58	16.927	2516	2522	2531	rVB2	35457	77755	4.81%	0.482%
59	17.374	2591	2598	2608	rBV	24874	60268	3.73%	0.373%

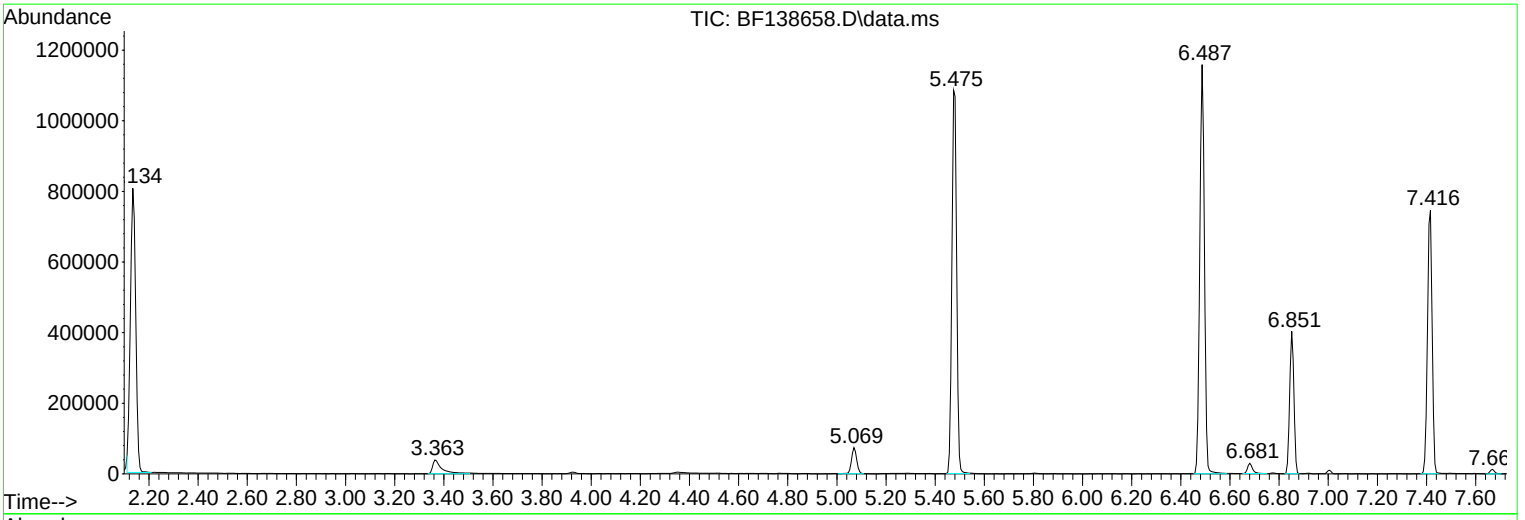
Sum of corrected areas: 16139169

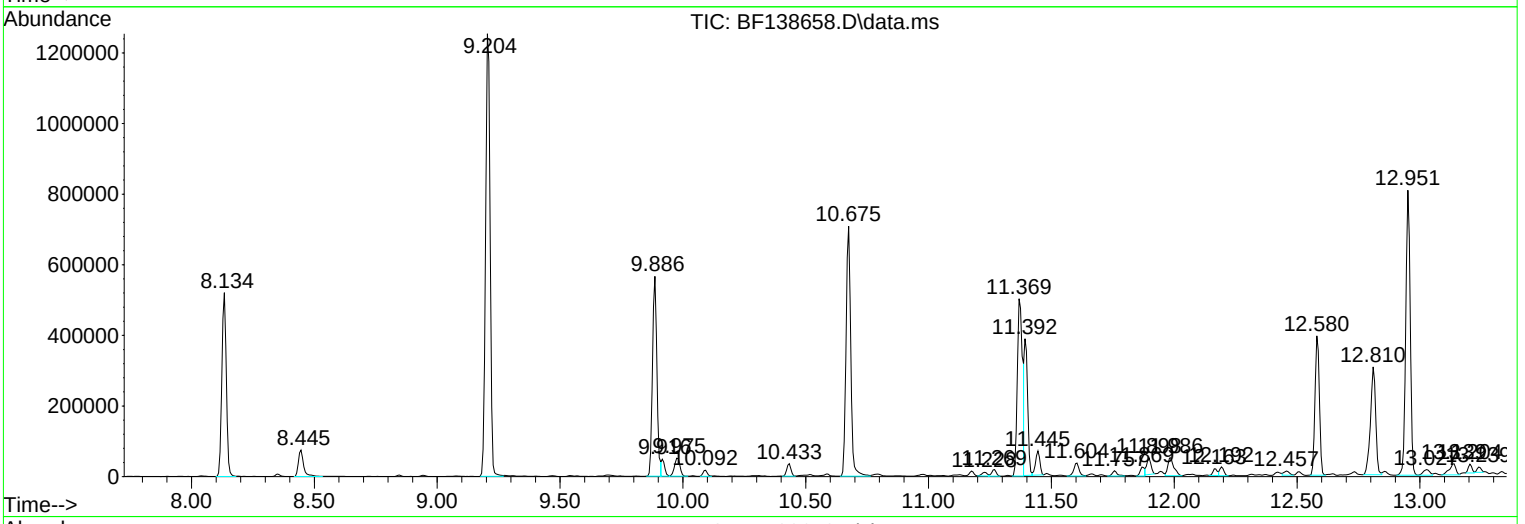
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
Data File : BF138658.D
Acq On : 25 Jul 2024 17:50
Operator : RC/JU
Sample : P3357-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

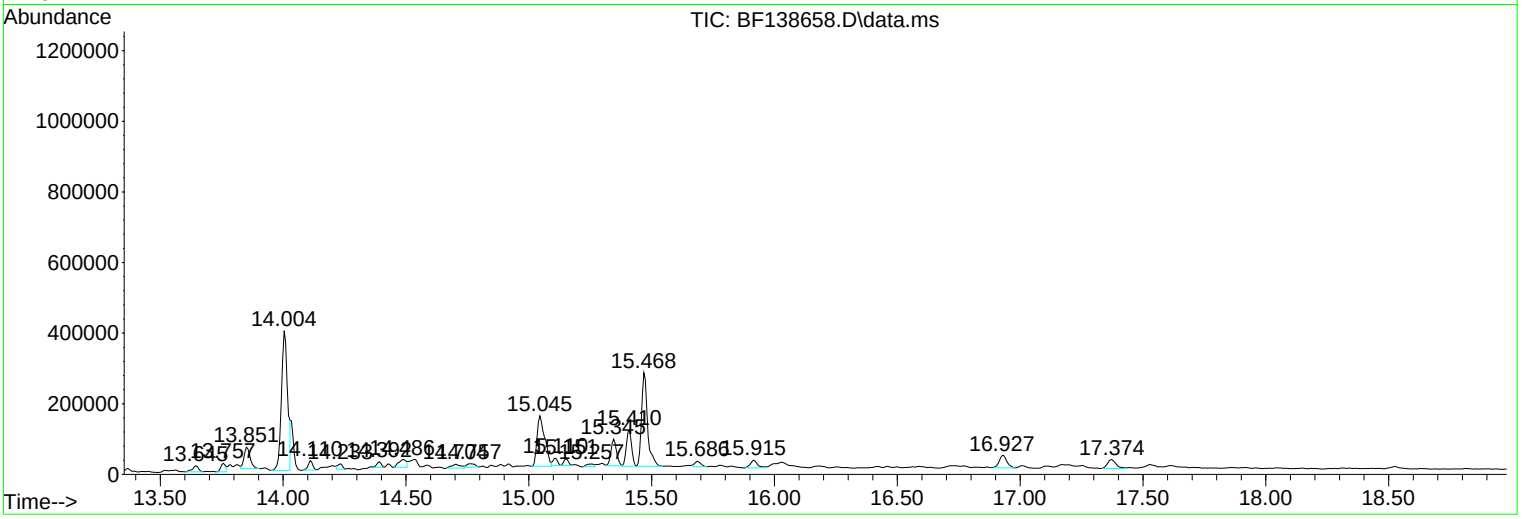
Instrument :
BNA_F
ClientSampleId :
S-857-J-SO-1-1.5-072024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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\BF072524\
Data File : BF138658.D
Acq On : 25 Jul 2024 17:50
Operator : RC/JU
Sample : P3357-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-857-J-SO-1-1.5-072024

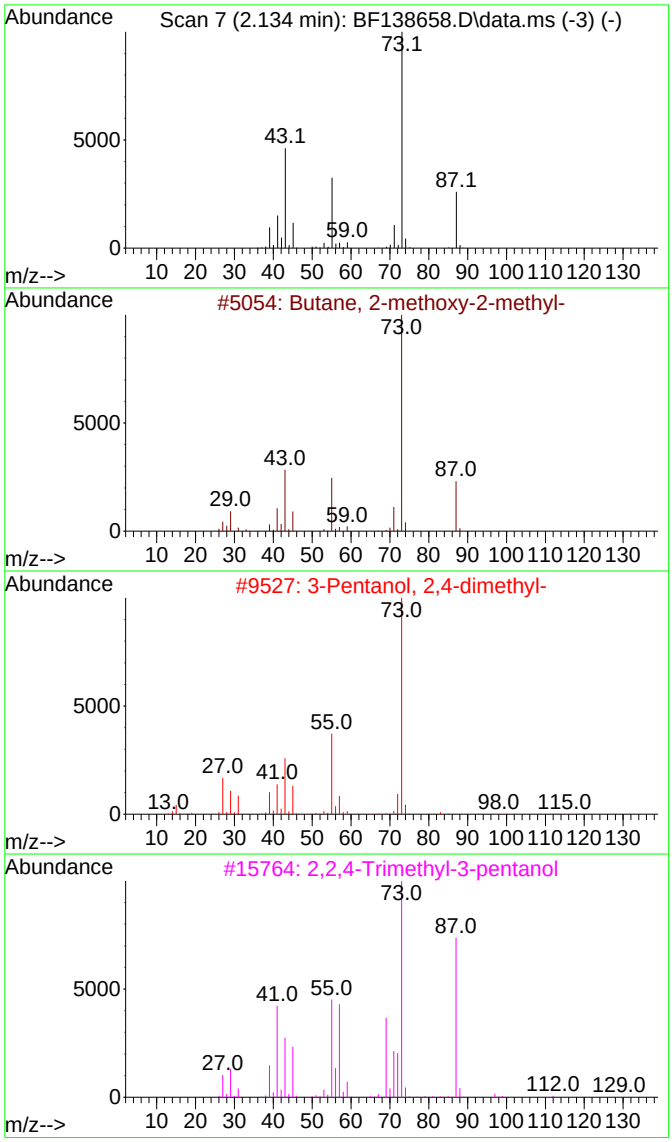
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

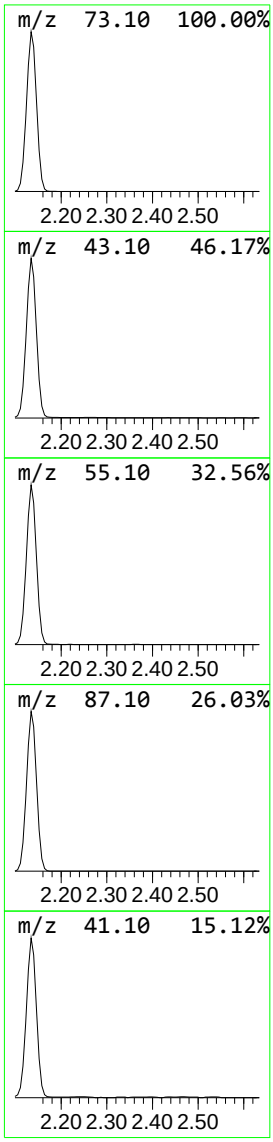
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	50.06 ng	1214710	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
Data File : BF138658.D
Acq On : 25 Jul 2024 17:50
Operator : RC/JU
Sample : P3357-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-857-J-SO-1-1.5-072024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

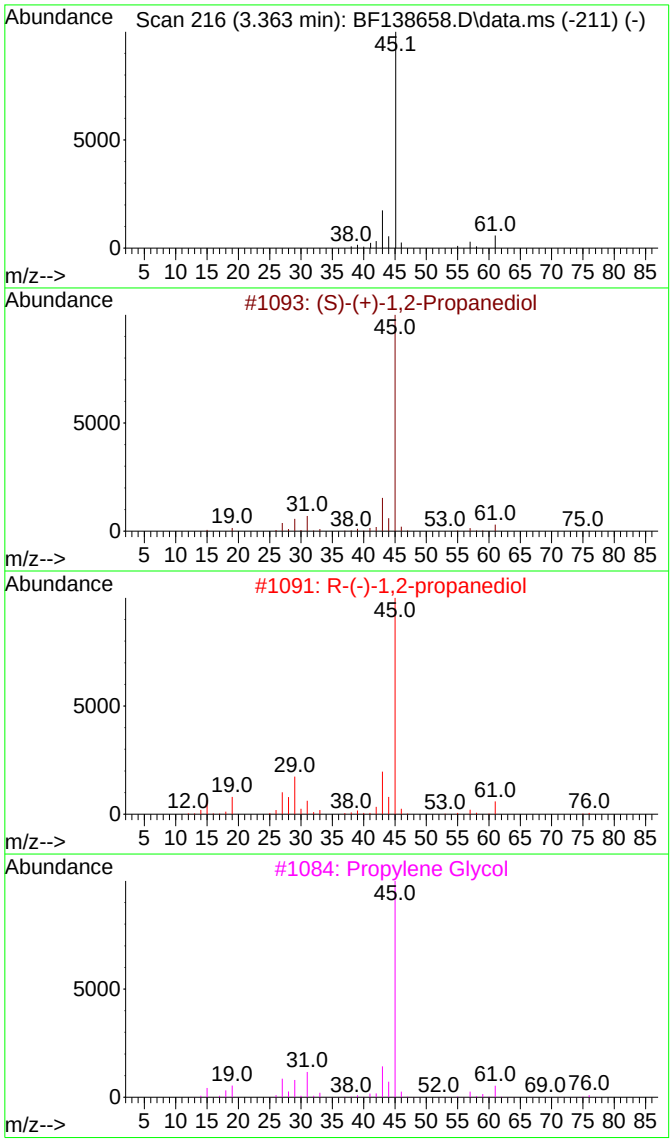
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

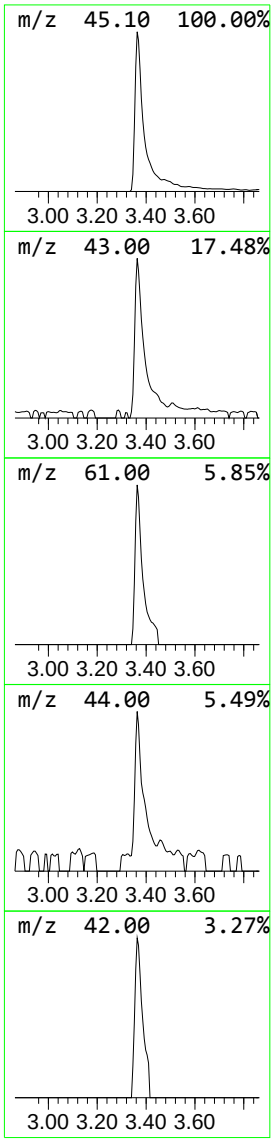
****

Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.363	4.23 ng	102744	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	74
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
Data File : BF138658.D
Acq On : 25 Jul 2024 17:50
Operator : RC/JU
Sample : P3357-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-857-J-SO-1-1.5-072024

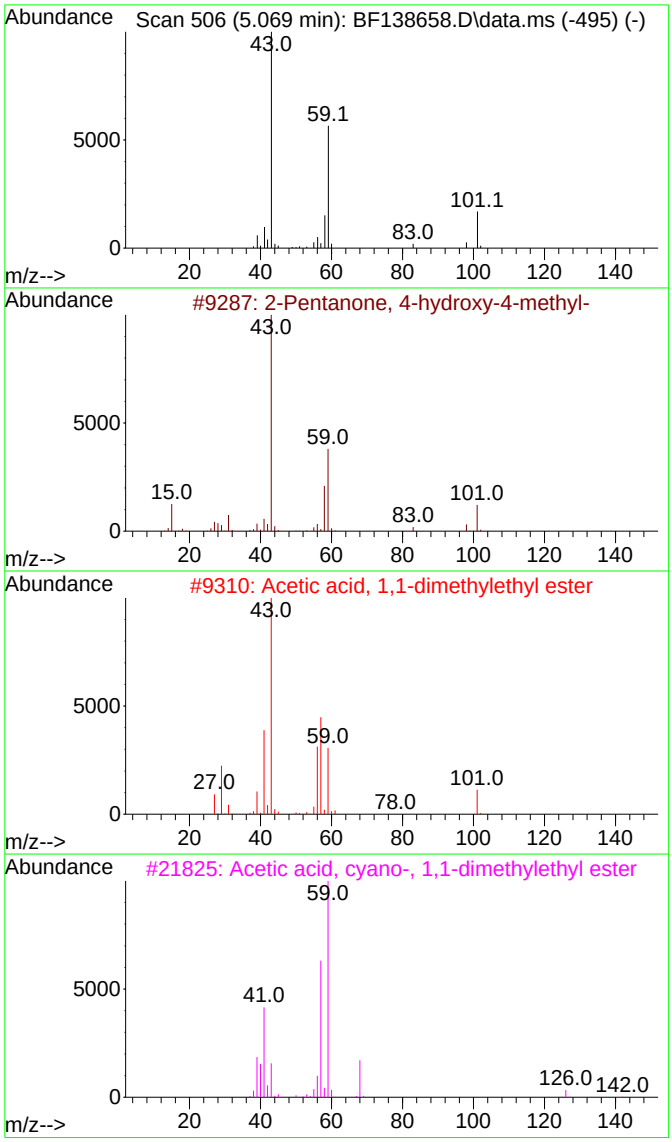
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

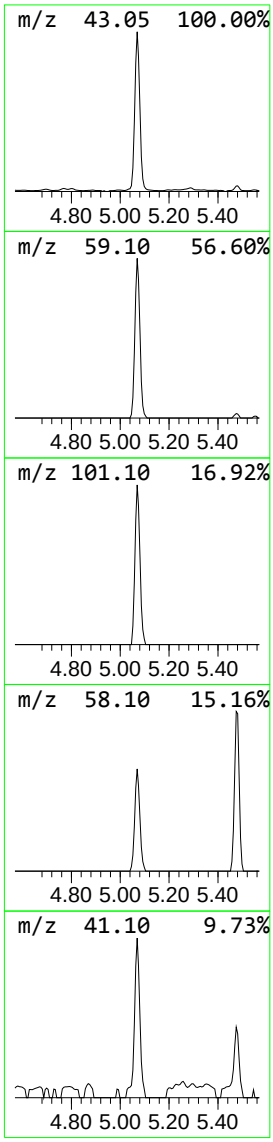
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	4.46 ng	108278	1,4-Dichlorobenzene-d4	6.851

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	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
Data File : BF138658.D
Acq On : 25 Jul 2024 17:50
Operator : RC/JU
Sample : P3357-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-857-J-SO-1-1.5-072024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

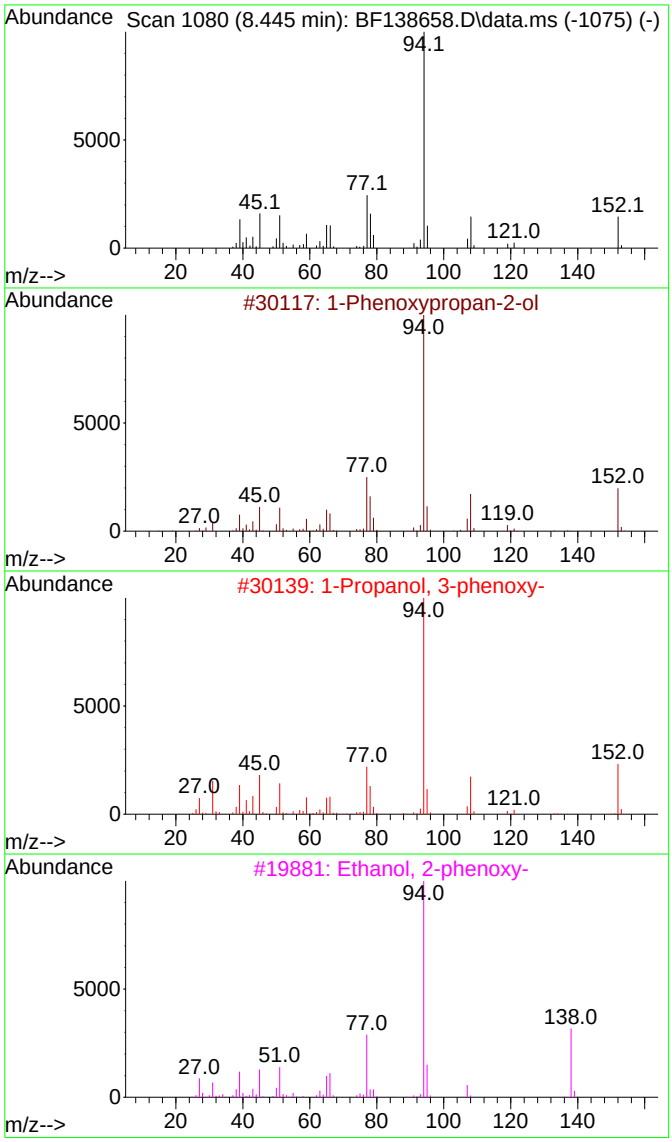
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

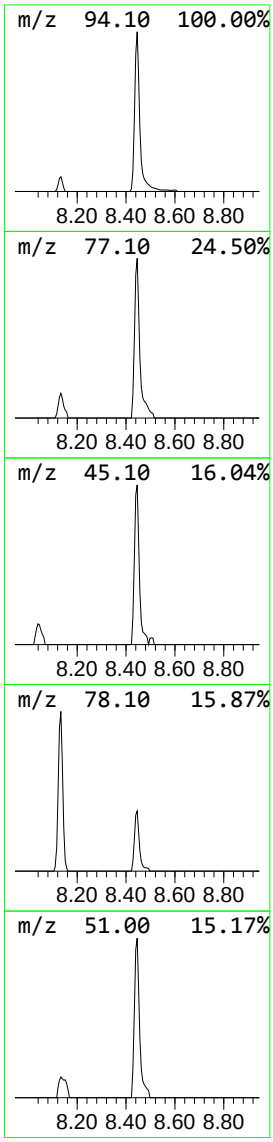
****

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.445	3.37 ng	110735	Naphthalene-d8	8.134

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	91
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
5	3-(.alpha.-Hydroxyethyl)-aniline	137	C8H11NO	002454-37-7	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
Data File : BF138658.D
Acq On : 25 Jul 2024 17:50
Operator : RC/JU
Sample : P3357-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-857-J-SO-1-1.5-072024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

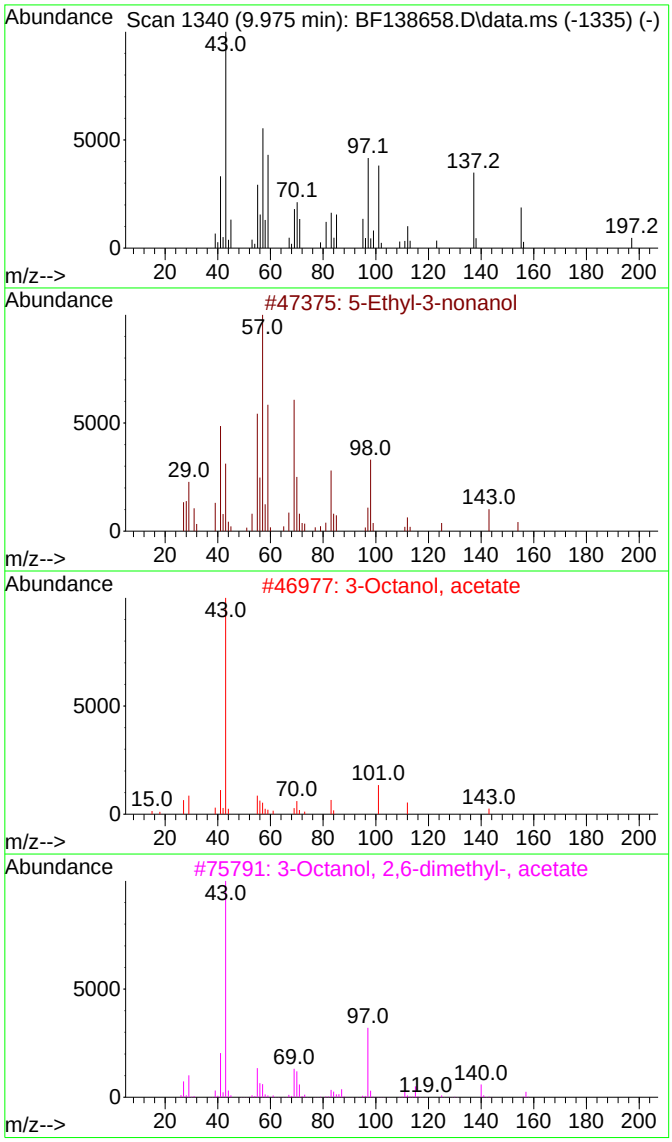
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

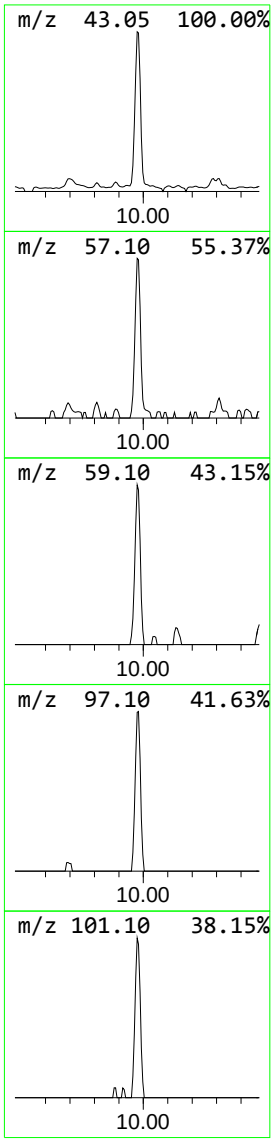
****

Peak Number 5 unknown9.975 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.975	2.23 ng	79799	Acenaphthene-d10	9.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Ethyl-3-nonanol	172	C11H24O	019780-71-3	22
2	3-Octanol, acetate	172	C10H20O2	004864-61-3	14
3	3-Octanol, 2,6-dimethyl-, acetate	200	C12H24O2	123232-57-5	14
4	Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	14
5	2-t-Butyl-5-methyl[1,3]dioxolan-...	158	C8H14O3	130930-47-1	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
Data File : BF138658.D
Acq On : 25 Jul 2024 17:50
Operator : RC/JU
Sample : P3357-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-857-J-SO-1-1.5-072024

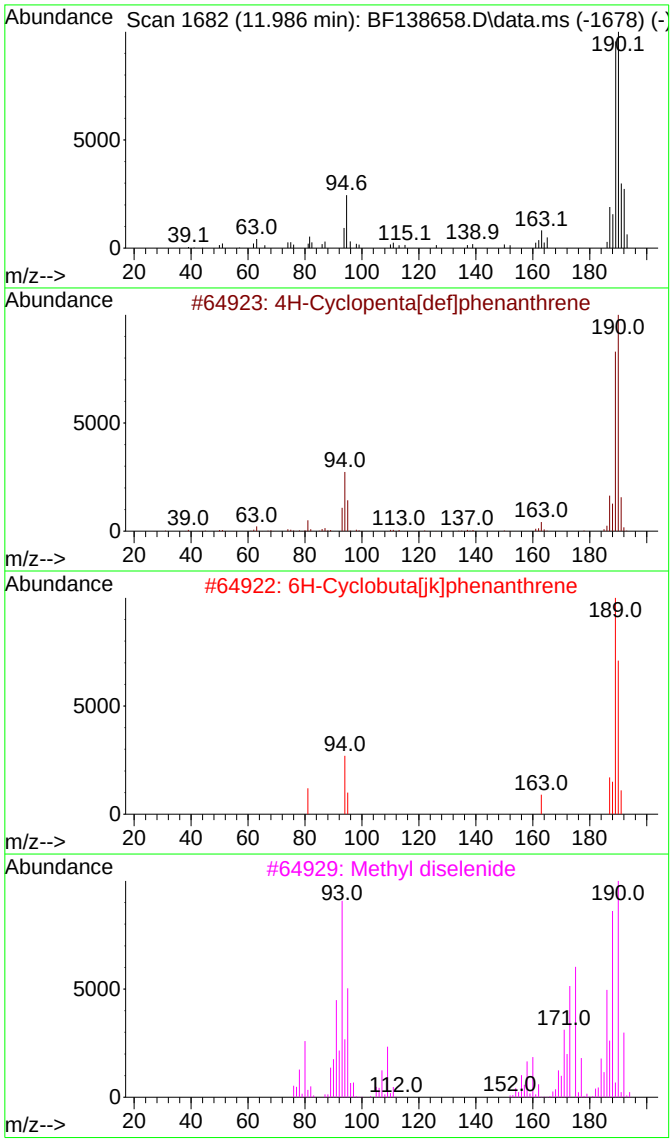
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

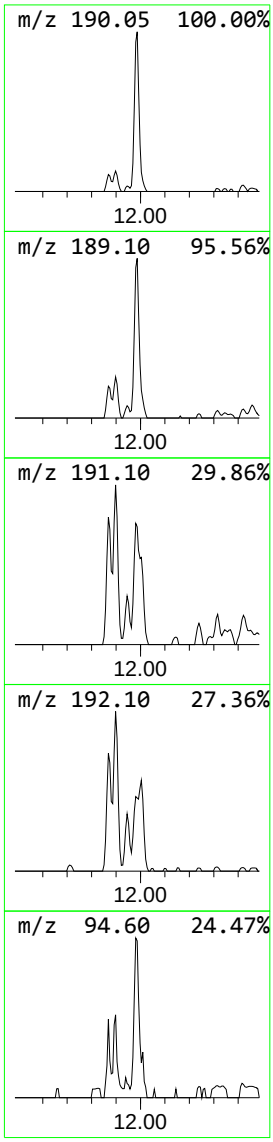
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.986	2.32 ng	86800	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3	Methyl diselenide	190	C2H6Se2	007101-31-7	49
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
5	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
Data File : BF138658.D
Acq On : 25 Jul 2024 17:50
Operator : RC/JU
Sample : P3357-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-857-J-SO-1-1.5-072024

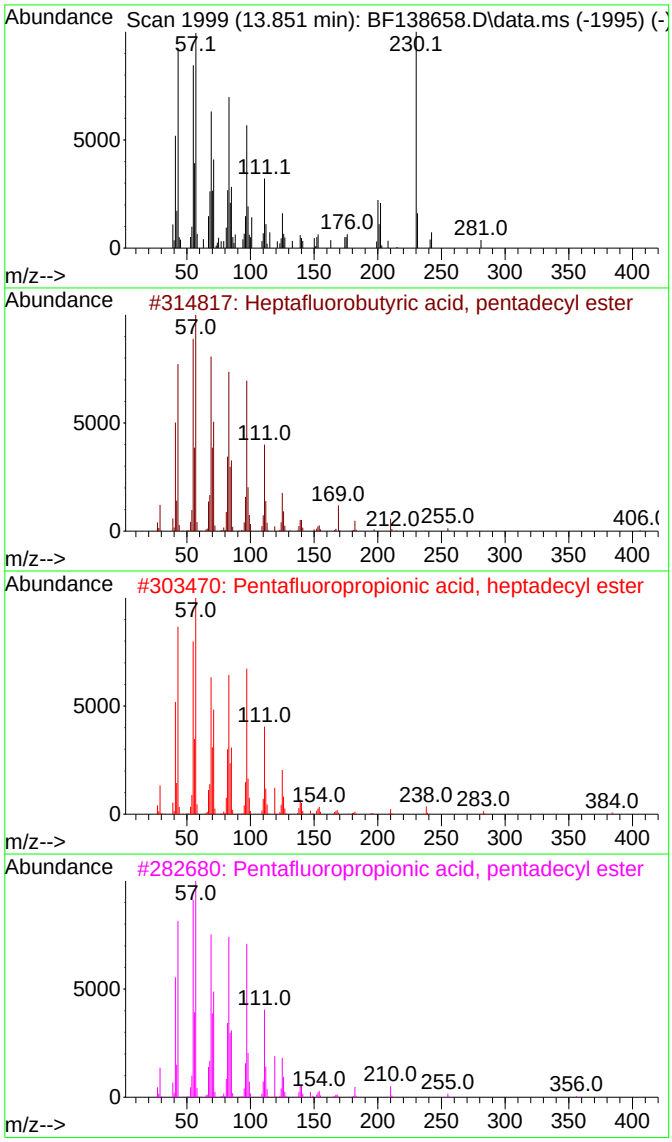
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

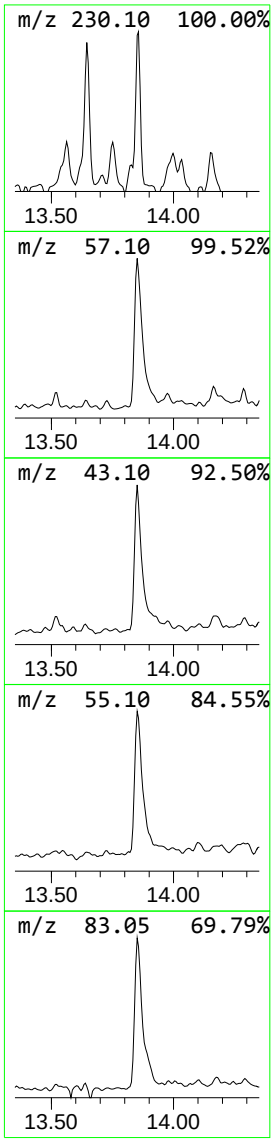
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Heptafluorobutyric acid, pe... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	2.99 ng	102389	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	90
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	90
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	90
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
Data File : BF138658.D
Acq On : 25 Jul 2024 17:50
Operator : RC/JU
Sample : P3357-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-857-J-SO-1-1.5-072024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

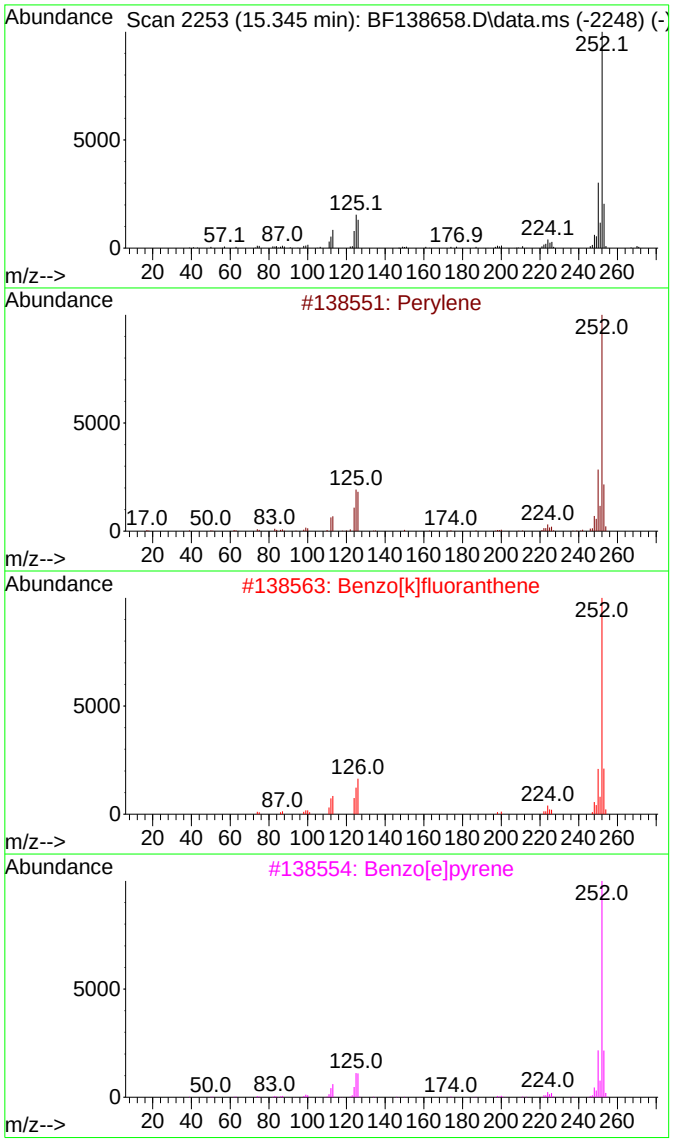
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

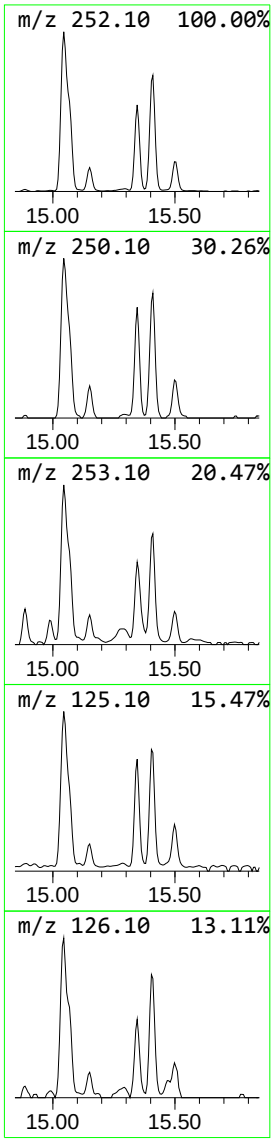
****

Peak Number 8 Perylene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.345	5.23 ng	117943	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	94
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
3	Benzo[e]pyrene	252	C20H12	000192-97-2	94
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Benzo[a]pyrene	252	C20H12	000050-32-8	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
Data File : BF138658.D
Acq On : 25 Jul 2024 17:50
Operator : RC/JU
Sample : P3357-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-857-J-SO-1-1.5-072024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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...	2.134	50.1	ng	1214710	1	6.851	485307	20.0
(S)-(+)-1,2-Pro...	3.363	4.2	ng	102744	1	6.851	485307	20.0
2-Pentanone, 4-...	5.069	4.5	ng	108278	1	6.851	485307	20.0
1-Phenoxypropan...	8.445	3.4	ng	110735	2	8.134	657943	20.0
unknown9.975	9.975	2.2	ng	79799	3	9.886	716613	20.0
4H-Cyclopenta[d...	11.986	2.3	ng	86800	4	11.369	748116	20.0
Heptafluorobuty...	13.851	3.0	ng	102389	5	14.010	685870	20.0
Perylene	15.345	5.2	ng	117943	6	15.468	450925	20.0