LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062322\
Data File : BF128971.D
Acq On : 24 Jun 2022 00:29
Operator : CG\JU
Sample : N3462-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6-4-6-20220622

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-BF060222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128971.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.928	445	449	460	rVB	84194	108580	4.21%	0.425%
2	5.357	519	522	541	rBV	2058488	2114131	82.04%	8.280%
3	6.387	693	697	710	rBV	2322342	2234056	86.70%	8.749%
4	6.722	751	754	760	rBV	682433	609726	23.66%	2.388%
5	7.292	846	851	854	rBV	1566273	1519387	58.96%	5.951%
6	8.010	967	973	975	rBV	879557	760649	29.52%	2.979%
7	8.028	975	976	981	rVB	115837	78891	3.06%	0.309%
8	8.722	1091	1094	1098	rVB	47350	37189	1.44%	0.146%
9	9.086	1151	1156	1159	rBV	3138292	2576909	100.00%	10.092%
10	9.357	1197	1202	1206	rBV2	40655	42993	1.67%	0.168%
11	9.763	1263	1271	1274	rBV	931243	751671	29.17%	2.944%
12	9.792	1274	1276	1280	rVB	159152	124326	4.82%	0.487%
13	9.969	1302	1306	1309	rBV	70345	60603	2.35%	0.237%
14	10.310	1361	1364	1369	rVB	115285	99232	3.85%	0.389%
15	10.551	1402	1405	1418	rBV	1075361	1023214	39.71%	4.007%
16	10.674	1422	1426	1434	rVB5	21014	36007	1.40%	0.141%
17	10.857	1450	1457	1460	rBV3	22720	30304	1.18%	0.119%
18	11.057	1488	1491	1495	rVB	53597	43088	1.67%	0.169%
19	11.110	1495	1500	1503	rVV3	22407	34149	1.33%	0.134%
20	11.145	1503	1506	1511	rVB	57530	51080	1.98%	0.200%
21	11.251	1520	1524	1526	rBV	722226	717104	27.83%	2.808%
22	11.274	1526	1528	1531	rVV	894260	674432	26.17%	2.641%
23	11.321	1531	1536	1540	rVB	200280	189763	7.36%	0.743%
24	11.486	1558	1564	1571	rBV2	123770	137268	5.33%	0.538%
25	11.645	1585	1591	1598	rVB2	75786	82944	3.22%	0.325%
26	11.751	1605	1609	1611	rBV	84914	73053	2.83%	0.286%
27	11.780	1611	1614	1618	rVV	132385	118442	4.60%	0.464%
28	11.827	1618	1622	1624	rVV	40461	41679	1.62%	0.163%
29	11.863	1624	1628	1630	rVV	154445	150731	5.85%	0.590%
30	11.886	1630	1632	1636	rVB	51595	43446	1.69%	0.170%
31	11.963	1637	1645	1647	rBV4	18445	41119	1.60%	0.161%
32	12.045	1656	1659	1662	rBV	65009	49562	1.92%	0.194%
33	12.074	1662	1664	1668	rVB	62450	56900	2.21%	0.223%
34	12.192	1679	1684	1688	rBV3	24290	34946	1.36%	0.137%
35	12.298	1699	1702	1705	rBV	37647	44544	1.73%	0.174%
36	12.339	1705	1709	1714	rVV6	41489	71219	2.76%	0.279%

LSC Area Percent Report

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Operator : CG\JU
Sample : N3462-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-6-4-6-20220622

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

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Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.392	1714	1718	1722	rVV3	52906	66429	2.58%	0.260%
38	12.463	1726	1730	1734	rVB	1199153	1044388	40.53%	4.090%
39	12.610	1751	1755	1759	rVB2	40187	57998	2.25%	0.227%
40	12.692	1763	1769	1775	rBV	955706	1021433	39.64%	4.000%
41	12.739	1775	1777	1780	rVB2	42911	39666	1.54%	0.155%
42	12.839	1786	1794	1797	rBV	2185783	2174261	84.37%	8.515%
43	12.910	1801	1806	1810	rBV2	59419	105067	4.08%	0.411%
44	12.998	1817	1821	1822	rBV3	64534	72027	2.80%	0.282%
45	13.021	1822	1825	1828	rVB	158857	142647	5.54%	0.559%
46	13.063	1828	1832	1833	rBV2	30068	38689	1.50%	0.152%
47	13.086	1833	1836	1839	rBV	124705	98767	3.83%	0.387%
48	13.121	1839	1842	1845	rBV2	90024	101594	3.94%	0.398%
49	13.215	1855	1858	1861	rVB	47143	38543	1.50%	0.151%
50	13.251	1861	1864	1867	rBV2	47294	57536	2.23%	0.225%
51	13.445	1895	1897	1900	rVB	40724	33871	1.31%	0.133%
52	13.533	1909	1912	1917	rVB	87076	84553	3.28%	0.331%
53	13.639	1927	1930	1932	rBV	131317	112364	4.36%	0.440%
54	13.668	1932	1935	1937	rVV	79858	68494	2.66%	0.268%
55	13.692	1937	1939	1941	rVV	62294	63949	2.48%	0.250%
56	13.745	1945	1948	1951	rBV	91224	96951	3.76%	0.380%
57	13.892	1965	1973	1976	rBV3	917577	1411922	54.79%	5.530%
58	13.921	1976	1978	1981	rVV	493643	393951	15.29%	1.543%
59	13.986	1985	1989	1994	rBV2	196415	273231	10.60%	1.070%
60	14.045	1996	1999	2004	rBV4	38156	69456	2.70%	0.272%
61	14.127	2011	2013	2015	rVB	56270	43885	1.70%	0.172%
62	14.239	2029	2032	2034	rBV2	58106	57851	2.24%	0.227%
63	14.280	2036	2039	2042	rVV	109611	105224	4.08%	0.412%
64	14.310	2042	2044	2049	rVB2	45676	46656	1.81%	0.183%
65	14.357	2049	2052	2054	rBV3	42961	54285	2.11%	0.213%
66	14.404	2058	2060	2062	rBV	55128	50307	1.95%	0.197%
67	14.592	2090	2092	2096	rBV2	40759	35295	1.37%	0.138%
68	14.762	2119	2121	2124	rBV2	44178	49481	1.92%	0.194%
69	14.921	2143	2148	2151	rBV	463857	723392	28.07%	2.833%
70	15.021	2162	2165	2169	rVB	81193	79557	3.09%	0.312%
71	15.209	2193	2197	2203	rVB	255439	341708	13.26%	1.338%
72	15.268	2203	2207	2212	rVB	362111	422449	16.39%	1.654%
73	15.327	2213	2217	2221	rBV	443499	565447	21.94%	2.215%
74	16.739	2451	2457	2462	rBV	136116	244852	9.50%	0.959%
75	17.162	2524	2529	2537	rVB2	89363	182225	7.07%	0.714%

LSC Area Percent Report

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Operator : CG\JU
Sample : N3462-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-6-4-6-20220622

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-BF060222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 25533738

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062322\
Data File : BF128971.D
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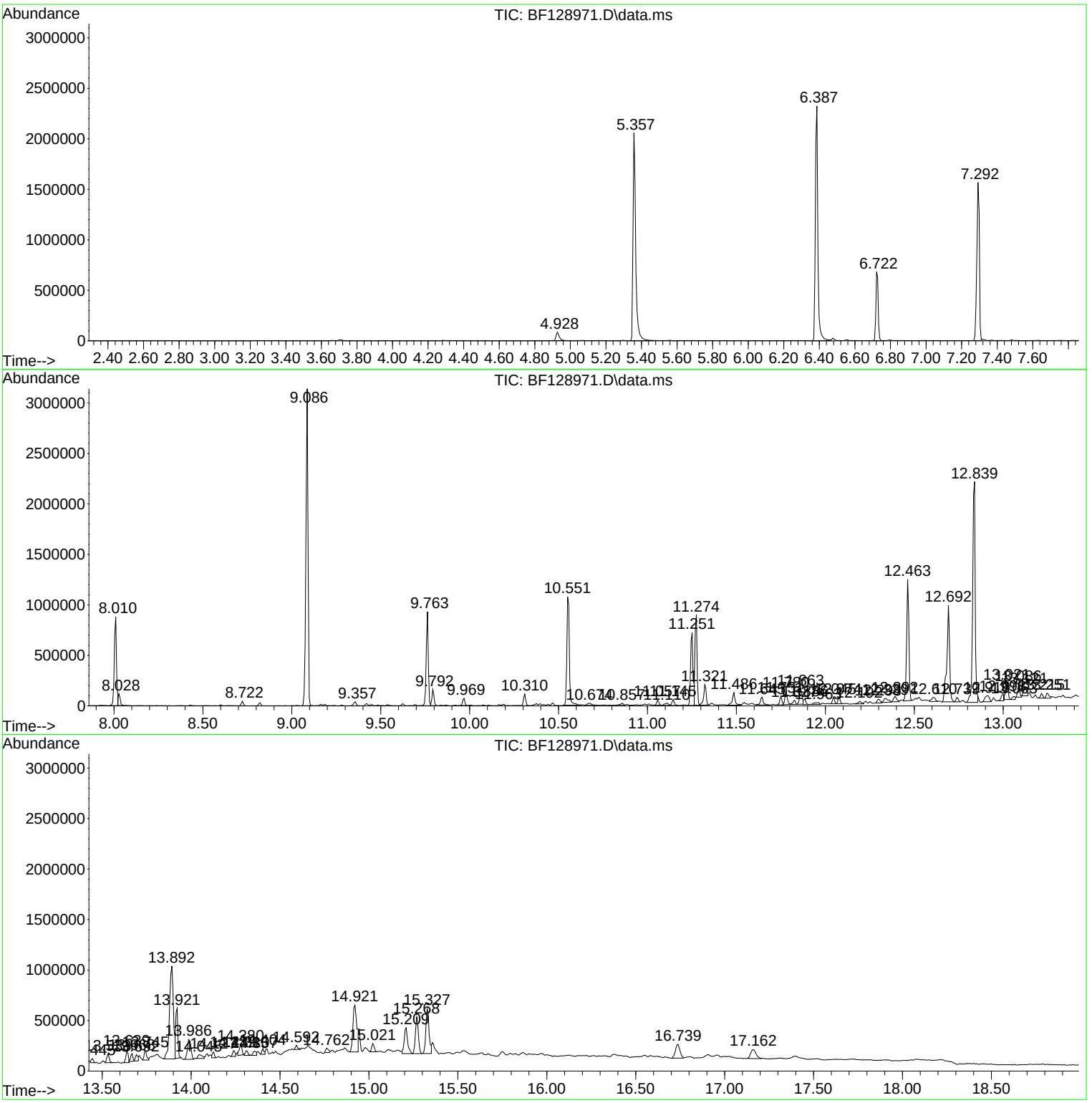
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-6-4-6-20220622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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\BF062322\
Data File : BF128971.D
Acq On : 24 Jun 2022 00:29
Operator : CG\JU
Sample : N3462-05
Misc :
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Instrument :
BNA_F
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SB-6-4-6-20220622

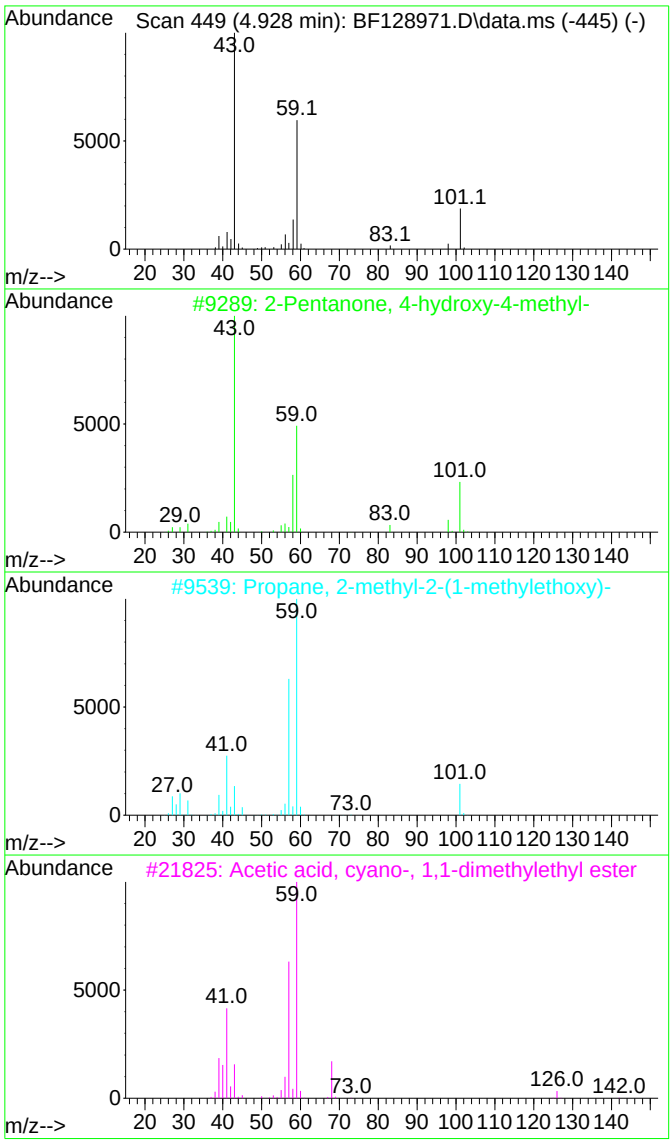
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

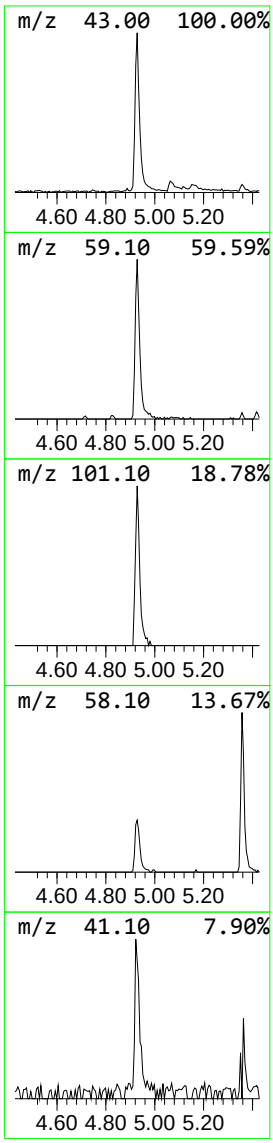
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.928	3.56 ng	108580	1,4-Dichlorobenzene-d4	6.728

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
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	Guanidine	59	CH5N3	000113-00-8	9





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

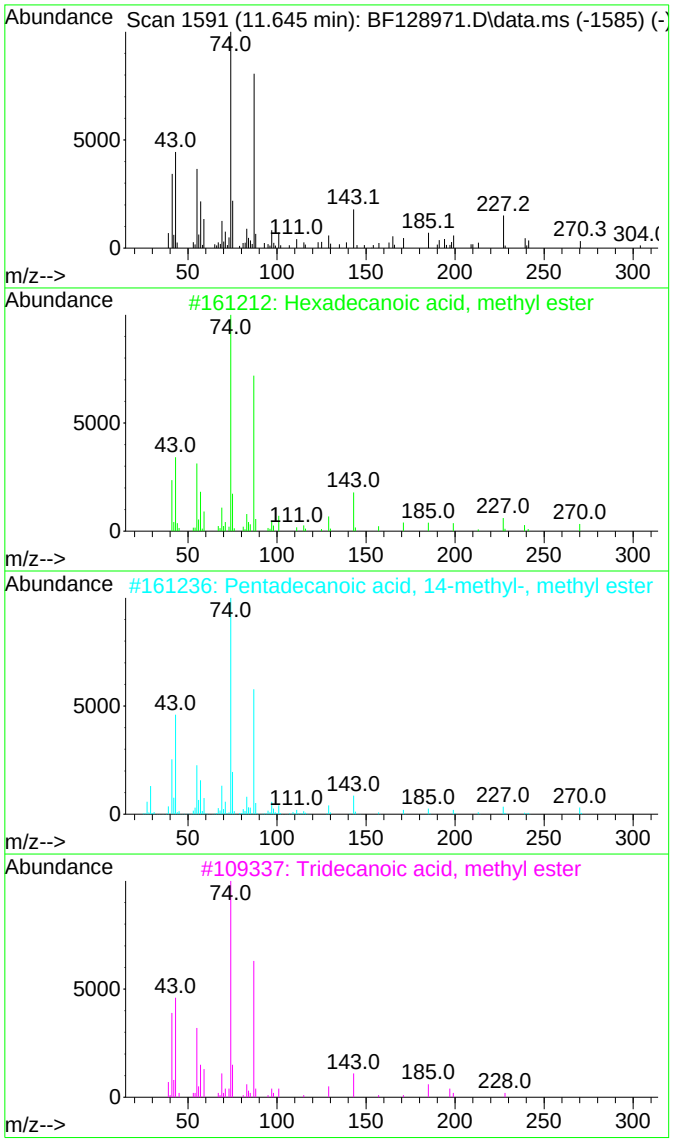
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

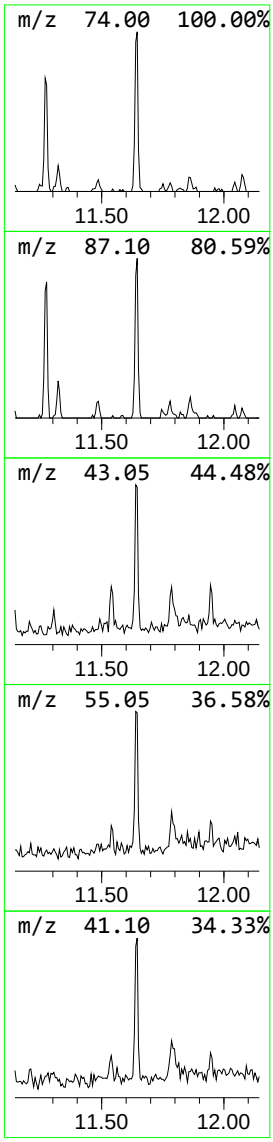
****

Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.645	2.31 ng	82944	Phenanthrene-d10	11.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	83
5	Methyl stearate	298	C19H38O2	000112-61-8	83





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Data File : BF128971.D
Acq On : 24 Jun 2022 00:29
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Sample : N3462-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

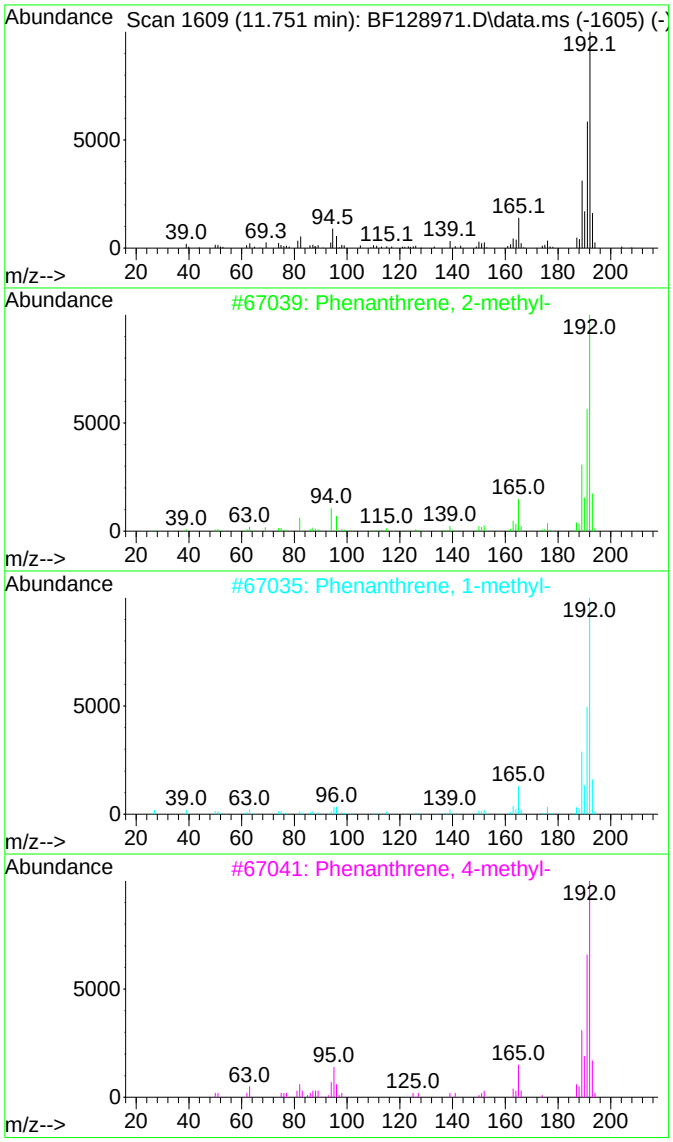
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

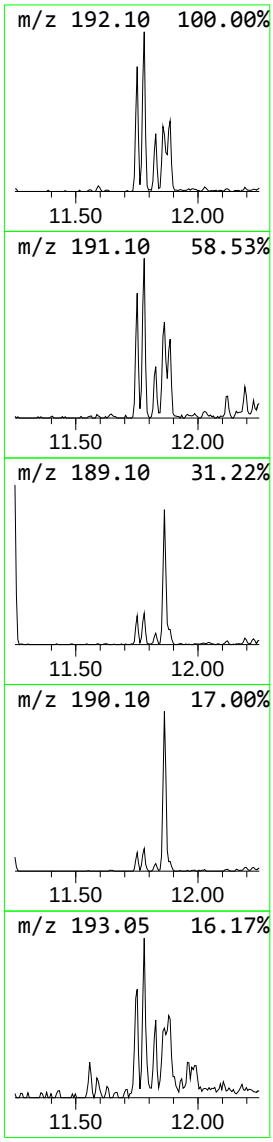
****

Peak Number 3 Phenanthrene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.751	2.04 ng	73053	Phenanthrene-d10	11.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	97
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	95
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	95
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	95





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

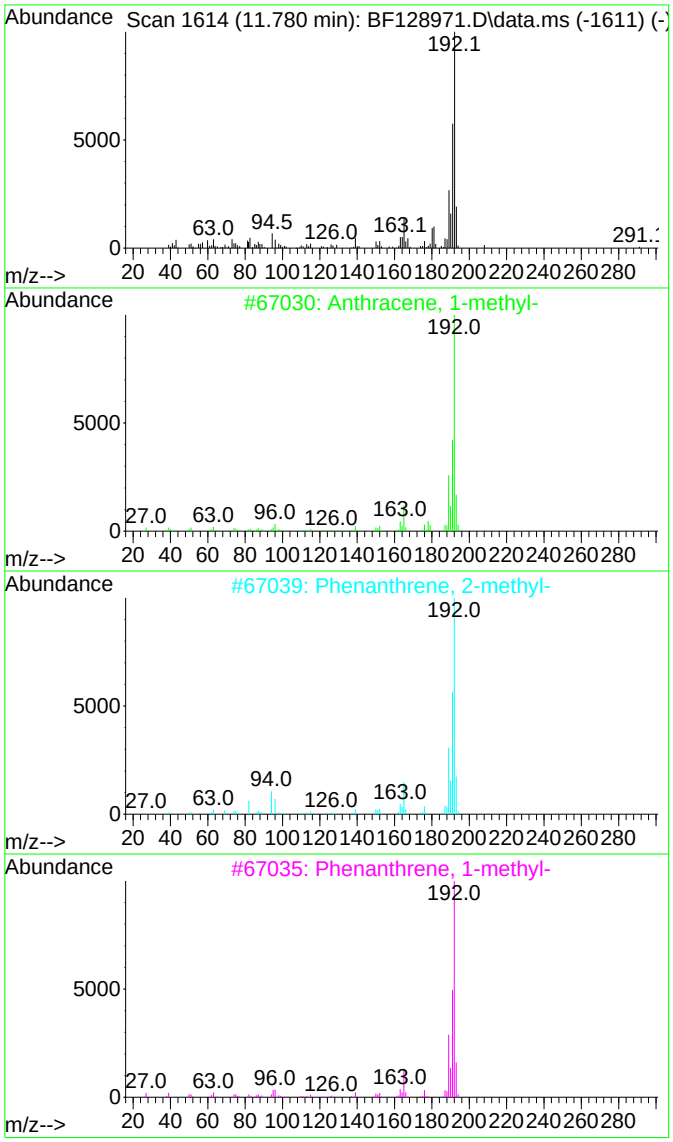
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

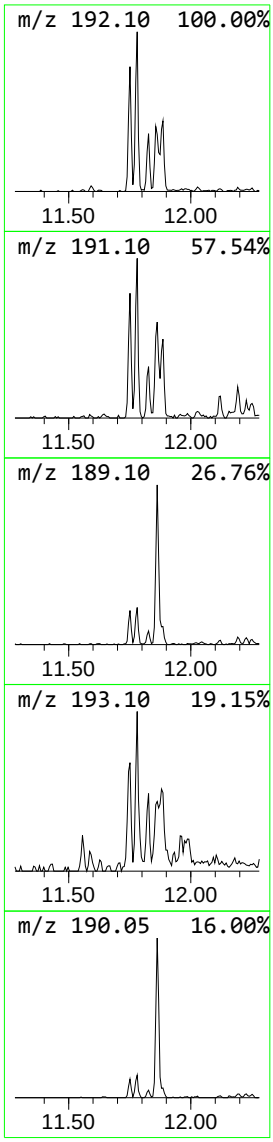
****

Peak Number 4 Anthracene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.780	3.30 ng	118442	Phenanthrene-d10	11.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	96
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	94
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	90





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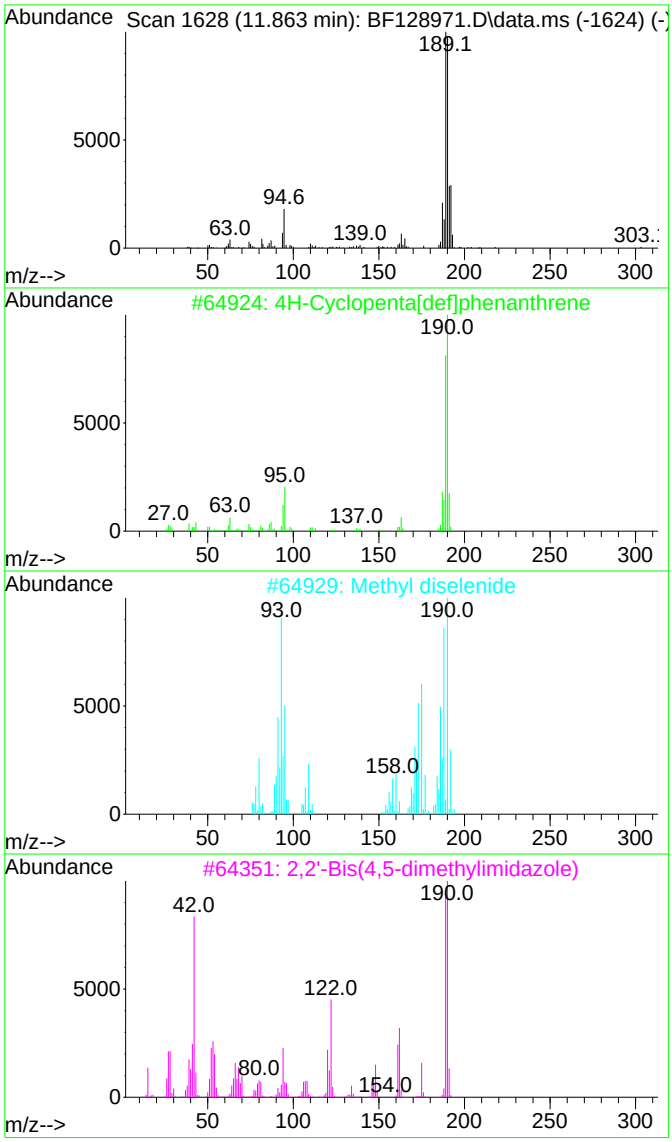
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

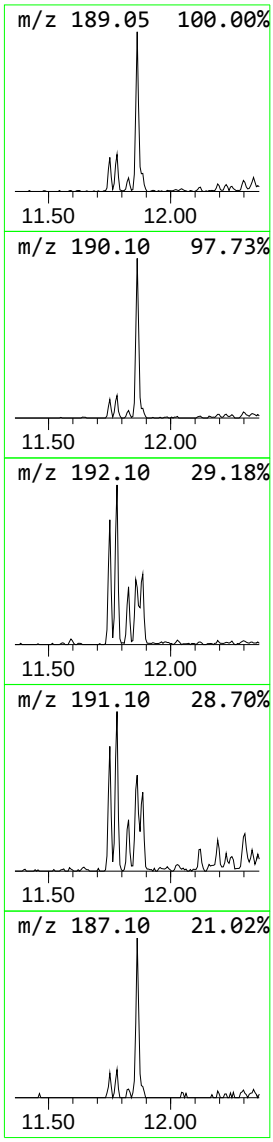
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	4.20 ng	150731	Phenanthrene-d10	11.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	Methyl diselenide	190	C2H6Se2	007101-31-7	49
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42
4	Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	27
5	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	25





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Data File : BF128971.D
Acq On : 24 Jun 2022 00:29
Operator : CG\JU
Sample : N3462-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-6-4-6-20220622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

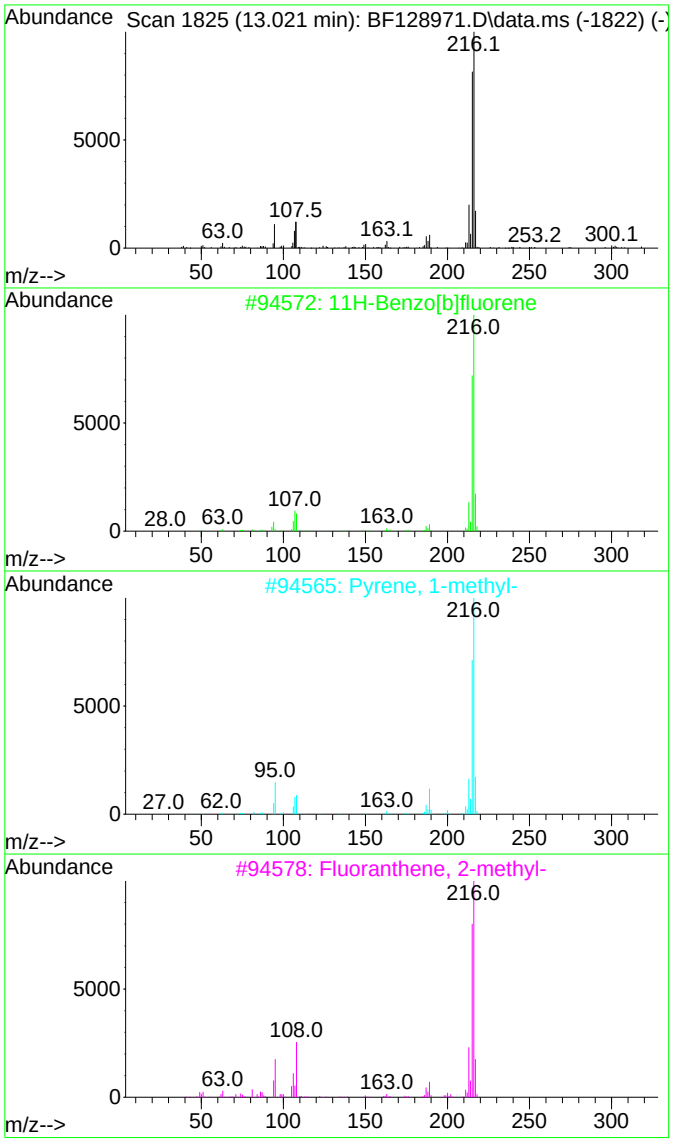
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

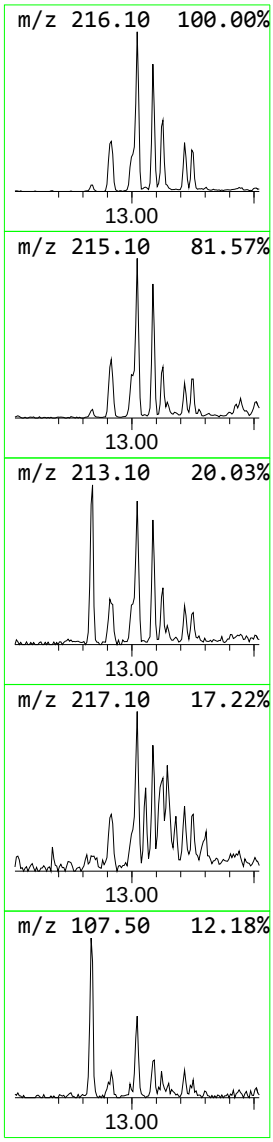
****

Peak Number 6 11H-Benzo[b]fluorene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.021	2.02 ng	142647	Chrysene-d12	13.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	81
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	81
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062322\
Data File : BF128971.D
Acq On : 24 Jun 2022 00:29
Operator : CG\JU
Sample : N3462-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-6-4-6-20220622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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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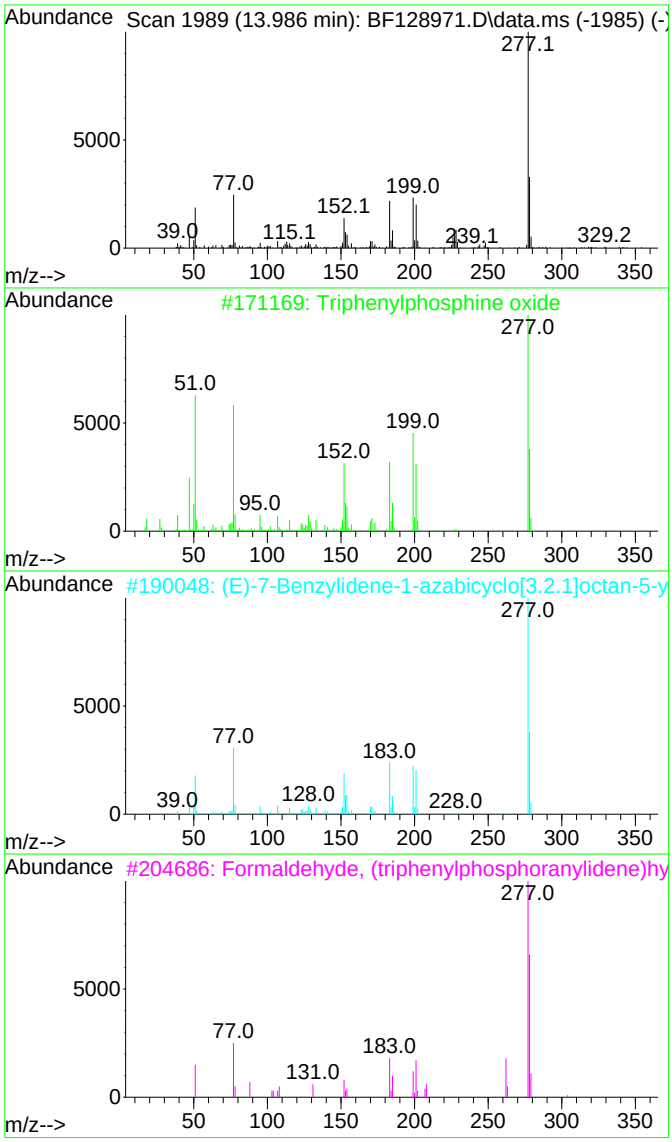
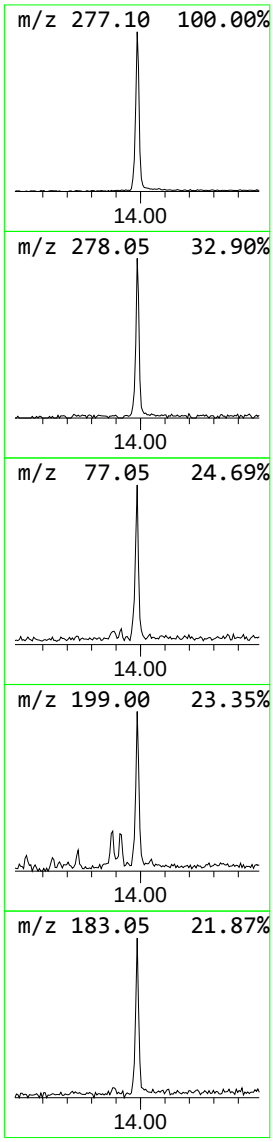
Peak Number 7 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.986	3.87 ng	273231	Chrysene-d12	13.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	38
5	5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062322\
Data File : BF128971.D
Acq On : 24 Jun 2022 00:29
Operator : CG\JU
Sample : N3462-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-6-4-6-20220622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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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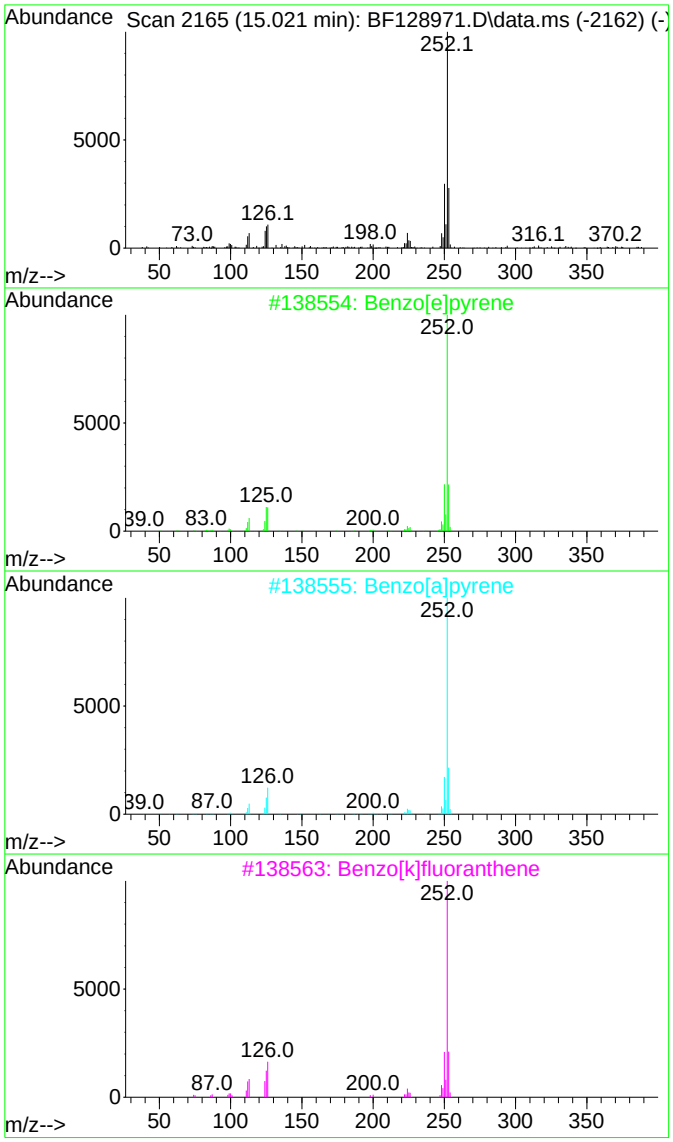
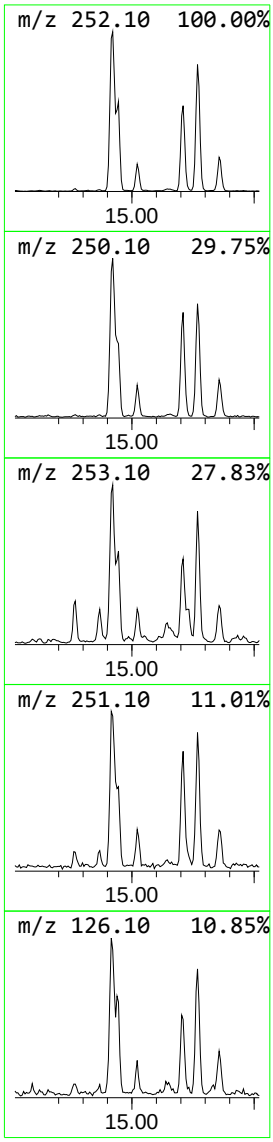
Peak Number 8 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.021	2.81 ng	79557	Perylene-d12	15.327

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	95
2	Benzo[a]pyrene	252	C20H12	000050-32-8	91
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	86
5	Perylene	252	C20H12	000198-55-0	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062322\
Data File : BF128971.D
Acq On : 24 Jun 2022 00:29
Operator : CG\JU
Sample : N3462-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-6-4-6-20220622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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
2-Pentanone, 4-...	4.928	3.6	ng	108580	1	6.728	609726	20.0
Hexadecanoic ac...	11.645	2.3	ng	82944	4	11.251	717104	20.0
Phenanthrene, 2...	11.751	2.0	ng	73053	4	11.251	717104	20.0
Anthracene, 1-m...	11.780	3.3	ng	118442	4	11.251	717104	20.0
4H-Cyclopenta[d...	11.863	4.2	ng	150731	4	11.251	717104	20.0
11H-Benzo[b]flu...	13.021	2.0	ng	142647	5	13.892	1411920	20.0
Triphenylphosph...	13.986	3.9	ng	273231	5	13.892	1411920	20.0
Benzo[e]pyrene	15.021	2.8	ng	79557	6	15.327	565447	20.0