LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
Data File : BF129828.D
Acq On : 17 Aug 2022 00:33
Operator : CG\JU
Sample : N4191-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-367

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-BF081422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129828.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.416	359	362	371	rBV	135199	175113	4.86%	0.607%
2	5.046	465	469	485	rVB	369699	460567	12.78%	1.596%
3	5.463	536	540	557	rBV	3041762	2899035	80.43%	10.043%
4	6.475	708	712	726	rBV	2976373	3061040	84.92%	10.605%
5	6.822	767	771	778	rBV	1000063	871749	24.18%	3.020%
6	7.387	863	867	871	rBV	2051794	2004838	55.62%	6.946%
7	8.104	985	989	992	rBV	1307398	1124035	31.18%	3.894%
8	9.175	1166	1171	1174	rBV	4089091	3604559	100.00%	12.488%
9	9.857	1281	1287	1290	rBV	1354369	1111337	30.83%	3.850%
10	9.892	1290	1293	1295	rVB	59084	53439	1.48%	0.185%
11	10.404	1376	1380	1385	rBV	49306	50692	1.41%	0.176%
12	10.651	1418	1422	1432	rBV	1521737	1334494	37.02%	4.623%
13	10.757	1436	1440	1443	rVV	37758	43703	1.21%	0.151%
14	11.345	1537	1540	1543	rBV	919128	874979	24.27%	3.031%
15	11.369	1543	1544	1548	rVV	391319	312463	8.67%	1.082%
16	11.422	1551	1553	1556	rVB	50737	46593	1.29%	0.161%
17	11.586	1576	1581	1584	rBV	63352	85629	2.38%	0.297%
18	11.851	1623	1626	1628	rBV	42366	43006	1.19%	0.149%
19	11.880	1628	1631	1636	rVB2	53530	60240	1.67%	0.209%
20	11.963	1642	1645	1647	rBV	76759	64561	1.79%	0.224%
21	12.180	1679	1682	1686	rVB	65517	56210	1.56%	0.195%
22	12.569	1744	1748	1751	rBV	878256	801210	22.23%	2.776%
23	12.798	1780	1787	1792	rBV	740102	797719	22.13%	2.764%
24	12.845	1792	1795	1799	rVB2	37240	41247	1.14%	0.143%
25	12.933	1806	1810	1813	rBV	2812128	2327088	64.56%	8.062%
26	13.016	1819	1824	1828	rBV3	40286	73284	2.03%	0.254%
27	13.127	1835	1843	1845	rBV2	84900	144552	4.01%	0.501%
28	13.192	1851	1854	1856	rVB	64371	55559	1.54%	0.192%
29	13.227	1856	1860	1862	rBV2	55259	62292	1.73%	0.216%
30	13.351	1879	1881	1885	rBV	33366	41283	1.15%	0.143%
31	13.639	1927	1930	1933	rVB	87196	72788	2.02%	0.252%
32	13.745	1945	1948	1950	rBV	106434	90925	2.52%	0.315%
33	13.769	1950	1952	1955	rVV	66992	60480	1.68%	0.210%
34	13.798	1955	1957	1962	rVV2	82320	140284	3.89%	0.486%
35	13.851	1962	1966	1974	rVB3	165816	297055	8.24%	1.029%
36	13.998	1986	1991	1994	rBV2	956687	1236949	34.32%	4.285%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
Data File : BF129828.D
Acq On : 17 Aug 2022 00:33
Operator : CG\JU
Sample : N4191-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-367

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-BF081422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.021	1994	1995	1999	rVB	474420	338153	9.38%	1.171%
38	14.104	2007	2009	2011	rVB	71400	52766	1.46%	0.183%
39	14.351	2048	2051	2053	rBV2	43625	49558	1.37%	0.172%
40	14.510	2076	2078	2080	rBV	47101	43220	1.20%	0.150%
41	14.604	2092	2094	2097	rBV2	48768	41509	1.15%	0.144%
42	14.880	2138	2141	2145	rBV2	96133	120366	3.34%	0.417%
43	15.039	2164	2168	2171	rBV	594440	857995	23.80%	2.972%
44	15.151	2184	2187	2190	rBV	100447	112298	3.12%	0.389%
45	15.345	2216	2220	2226	rVB	333332	396016	10.99%	1.372%
46	15.404	2226	2230	2235	rVV	409910	530218	14.71%	1.837%
47	15.468	2237	2241	2244	rVV	640963	795769	22.08%	2.757%
48	15.498	2244	2246	2253	rVB	126955	172463	4.78%	0.597%
49	16.945	2486	2492	2500	rVB	230125	443539	12.30%	1.537%
50	17.398	2563	2569	2578	rVB	151993	330229	9.16%	1.144%

Sum of corrected areas: 28865096

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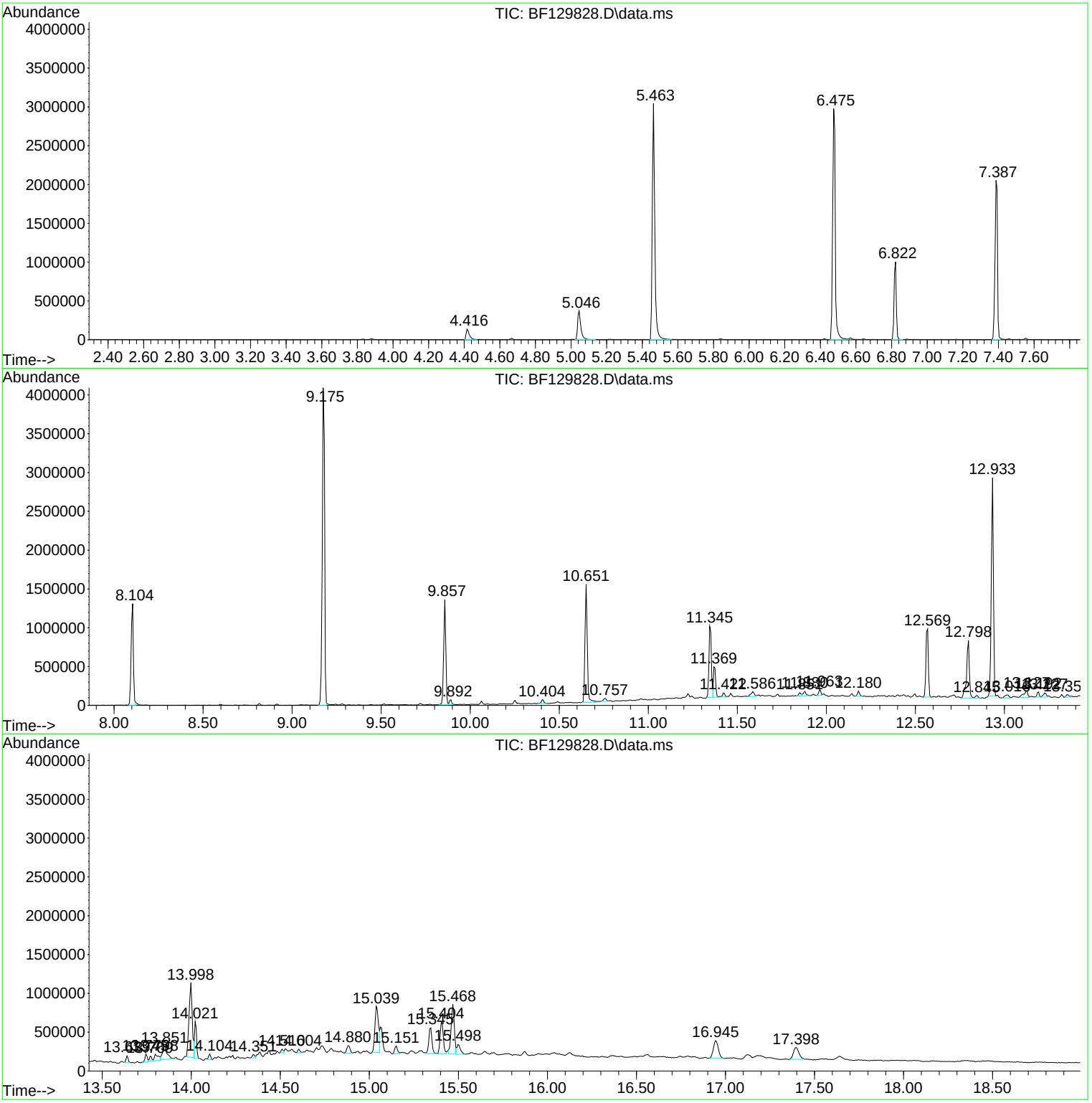
Instrument :
BNA_F
ClientSampleId :
RO-367

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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\BF081622\
Data File : BF129828.D
Acq On : 17 Aug 2022 00:33
Operator : CG\JU
Sample : N4191-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-367

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

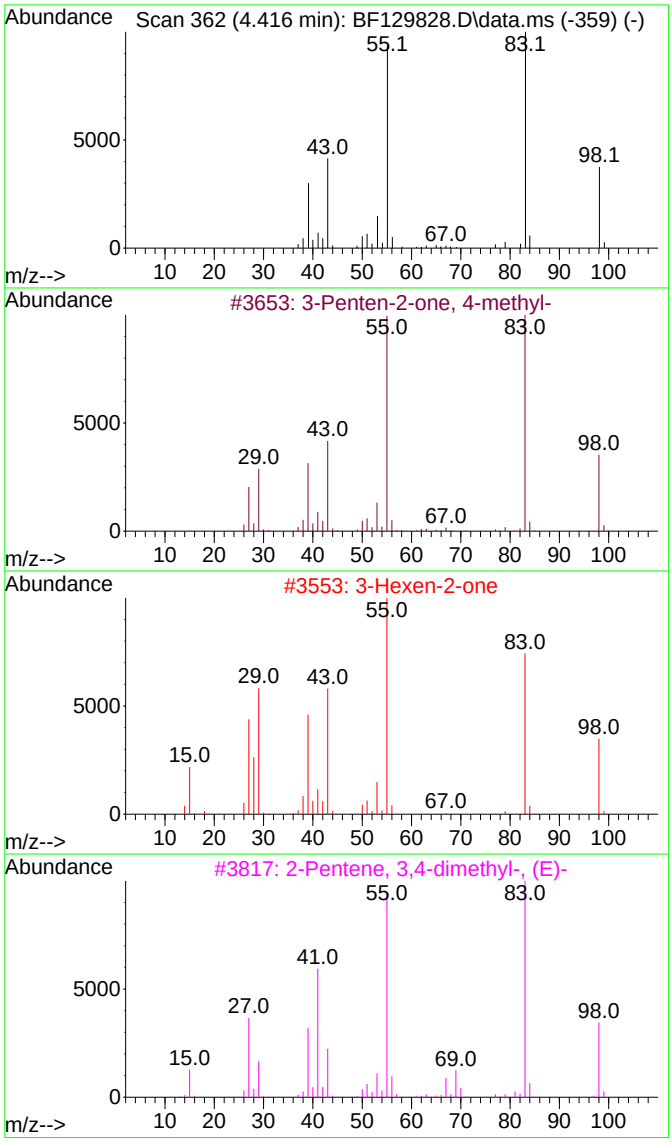
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

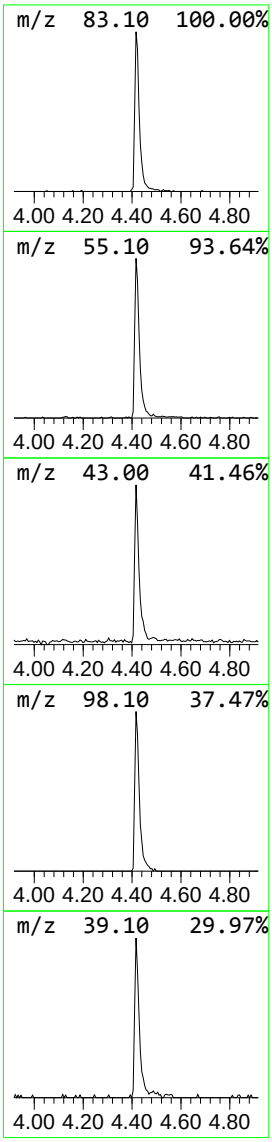
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.416	4.02 ng	175113	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
Data File : BF129828.D
Acq On : 17 Aug 2022 00:33
Operator : CG\JU
Sample : N4191-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-367

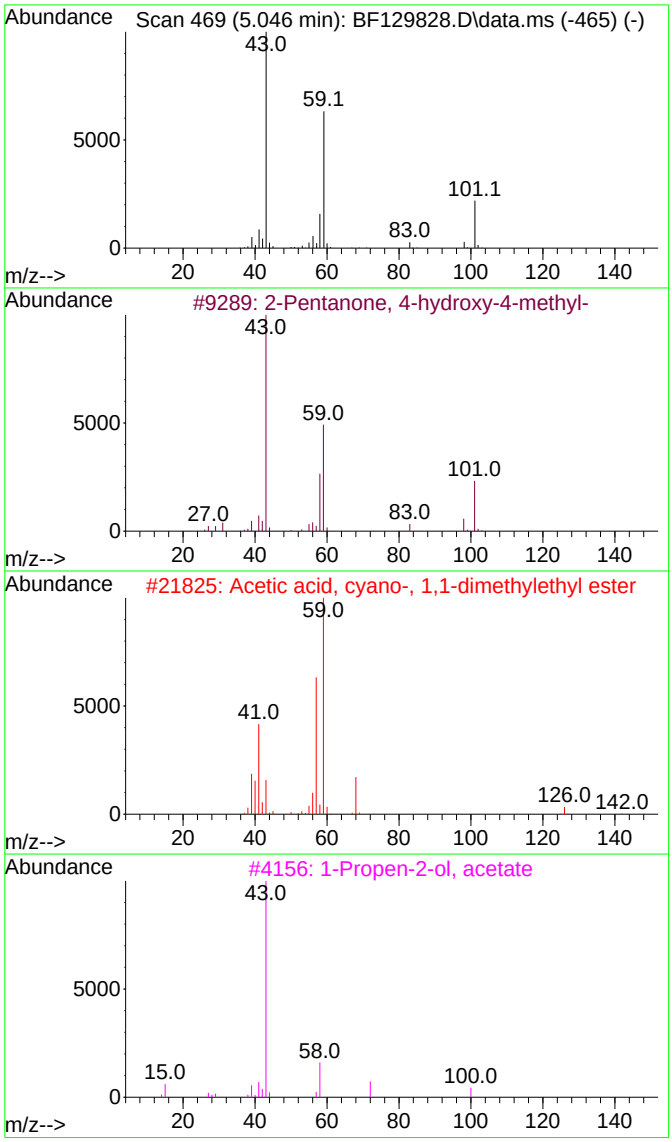
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

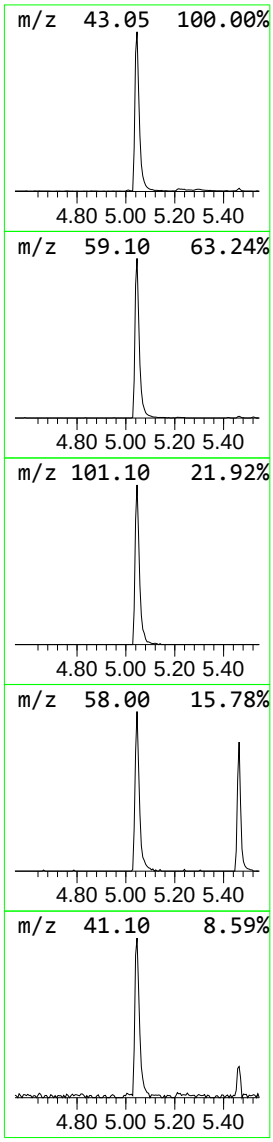
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.046	10.57 ng	460567	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Guanidine	59	CH5N3	000113-00-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
Data File : BF129828.D
Acq On : 17 Aug 2022 00:33
Operator : CG\JU
Sample : N4191-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-367

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

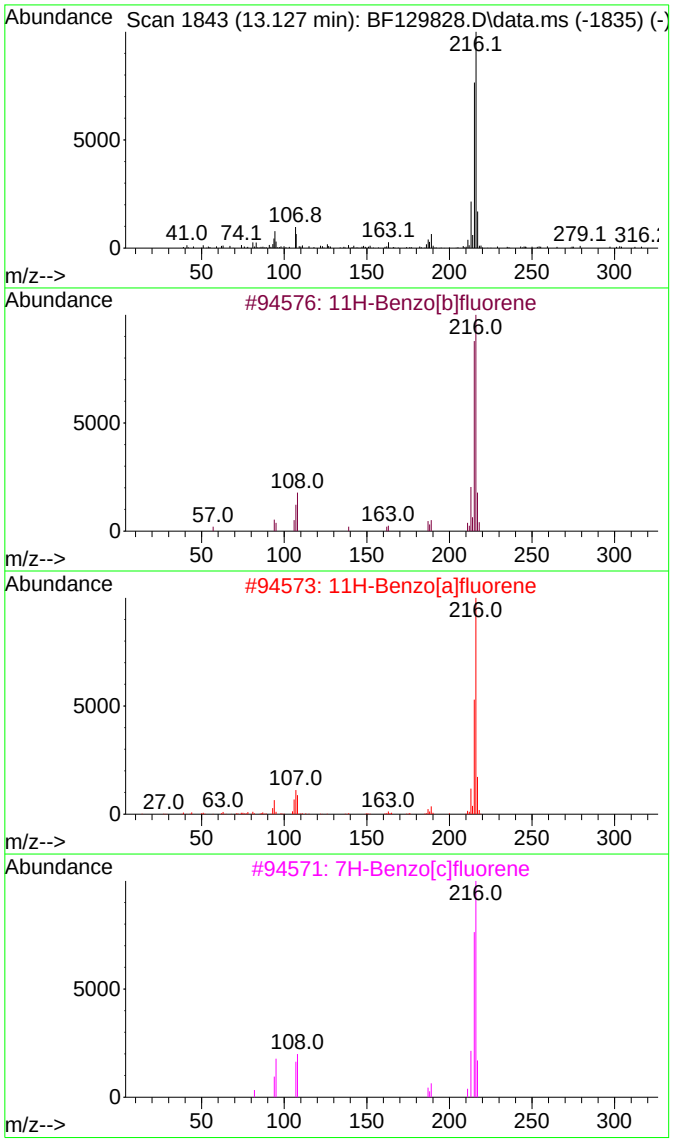
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

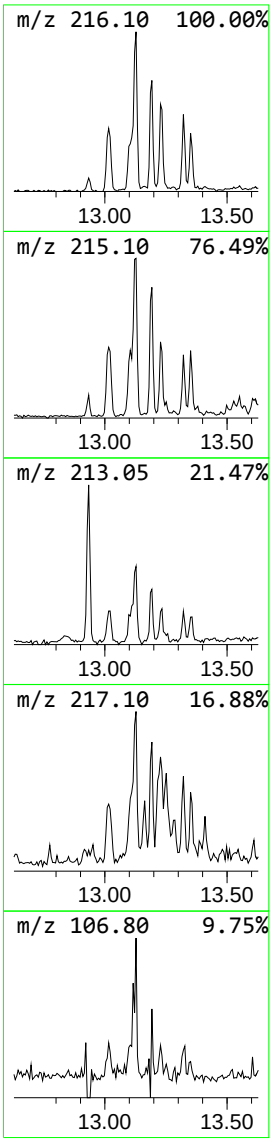
****

Peak Number 3 11H-Benzo[b]fluorene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.127	2.34 ng	144552	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
3	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	87
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
Data File : BF129828.D
Acq On : 17 Aug 2022 00:33
Operator : CG\JU
Sample : N4191-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-367

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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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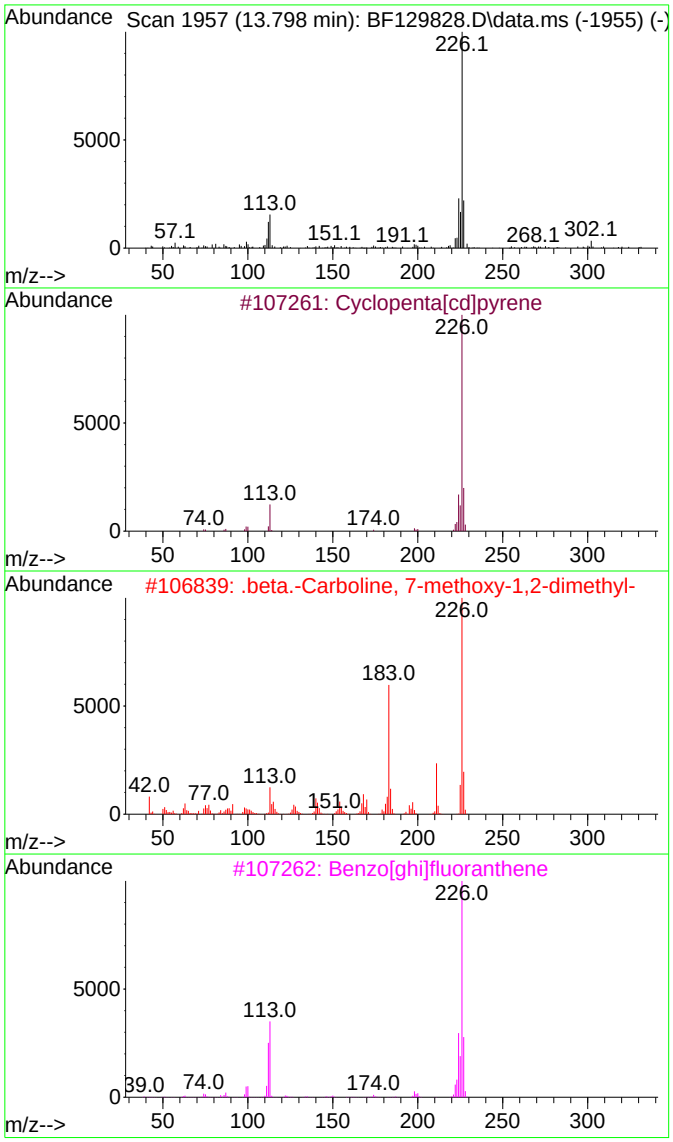
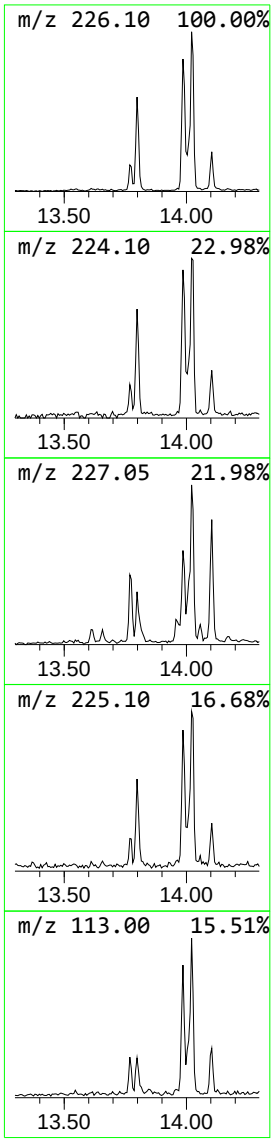
Peak Number 4 Cyclopenta[cd]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.798	2.27 ng	140284	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta[cd]pyrene	226	C18H10	027208-37-3	81
2	.beta.-Carboline, 7-methoxy-1,2-...	226	C14H14N2O	006519-18-2	58
3	Benzo[ghi]fluoranthene	226	C18H10	000203-12-3	53
4	1,3-Diamino-5,6-dihydro-7-methyl...	226	C13H14N4	037436-37-6	53
5	9H-Thioxanthen-9-one, 2-methyl-	226	C14H10OS	015774-82-0	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
Data File : BF129828.D
Acq On : 17 Aug 2022 00:33
Operator : CG\JU
Sample : N4191-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-367

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

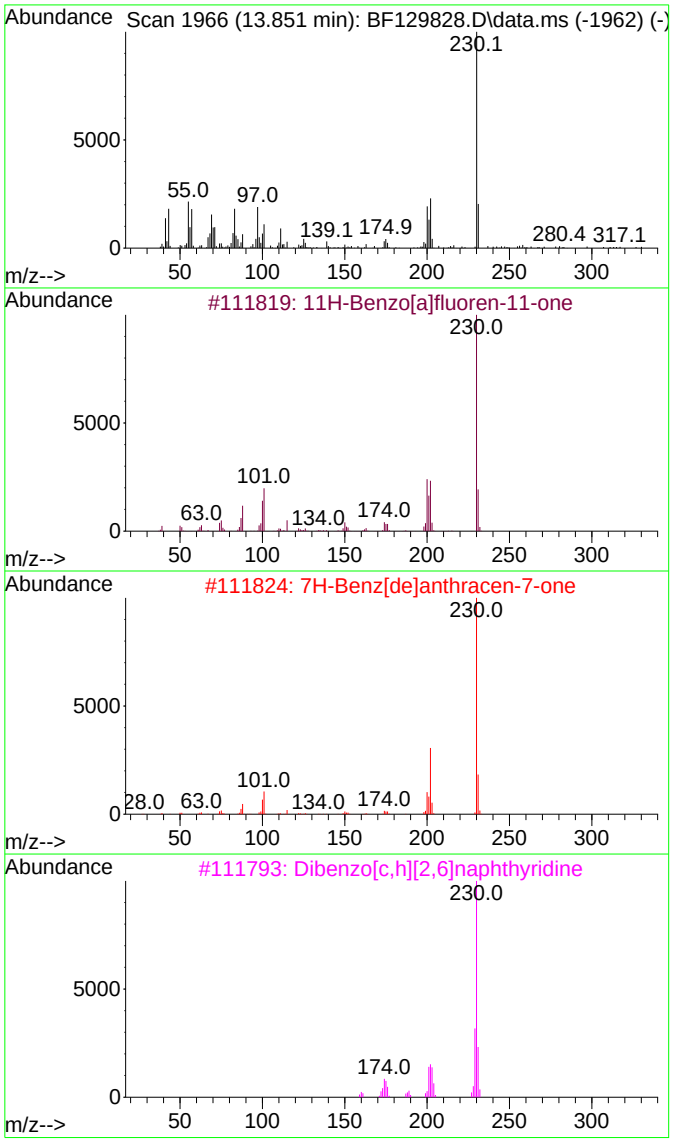
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

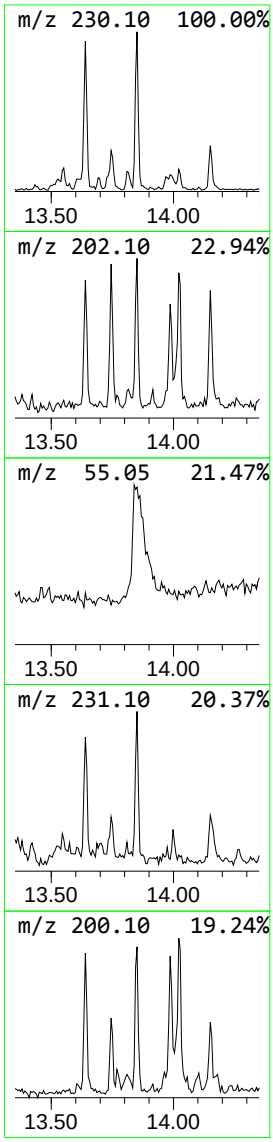
****

Peak Number 5 11H-Benzo[a]fluoren-11-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	4.80 ng	297055	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	91
2	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	76
3	Dibenzo[c,h][2,6]naphthyridine	230	C16H10N2	000218-30-4	64
4	6,6-Diphenylfulvene	230	C18H14	002175-90-8	53
5	o-Terphenyl	230	C18H14	000084-15-1	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
Data File : BF129828.D
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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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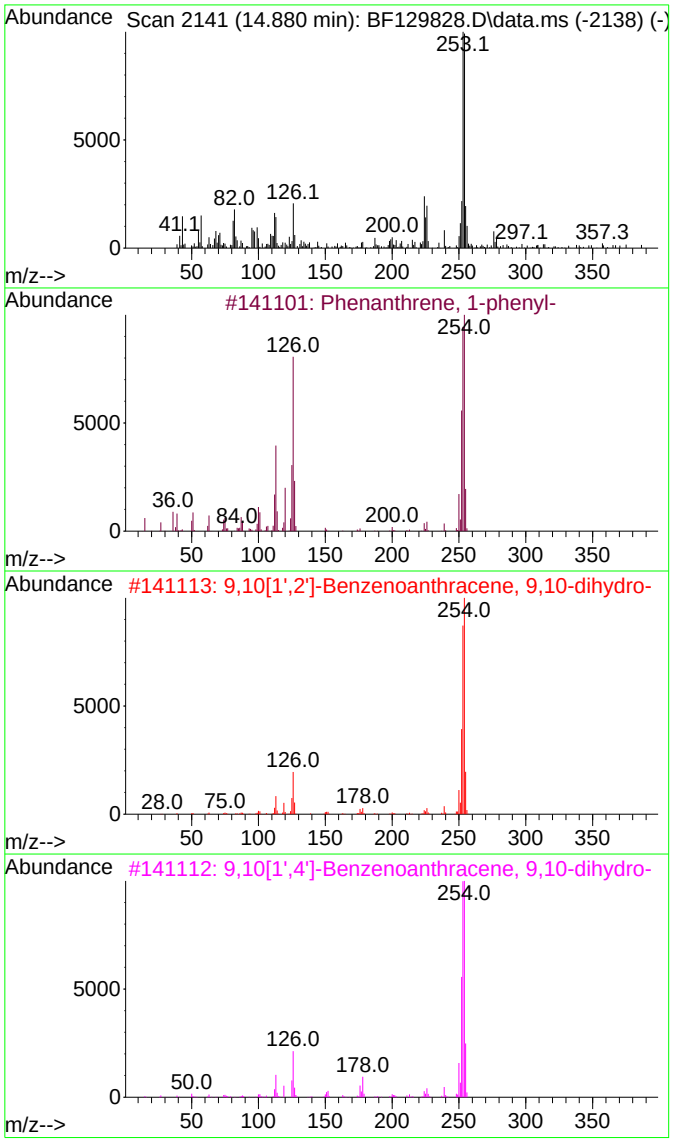
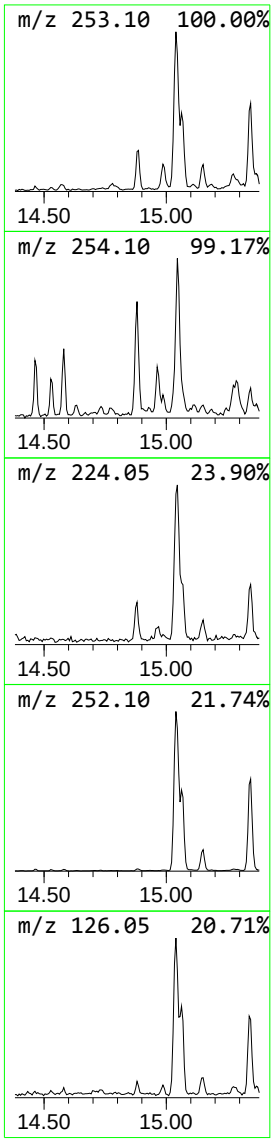
Peak Number 6 Phenanthrene, 1-phenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.880	3.03 ng	120366	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-phenyl-	254	C20H14	004325-76-2	68
2	9,10[1',2']-Benzenoanthracene, 9...	254	C20H14	000477-75-8	68
3	9,10[1',4']-Benzenoanthracene, 9...	254	C20H14	1000487-02-7	62
4	1,2'-Binaphthalene	254	C20H14	004325-74-0	62
5	4,5-Dihydrobenzo[e]pyrene	254	C20H14	095676-42-9	58





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Data File : BF129828.D
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Operator : CG\JU
Sample : N4191-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-367

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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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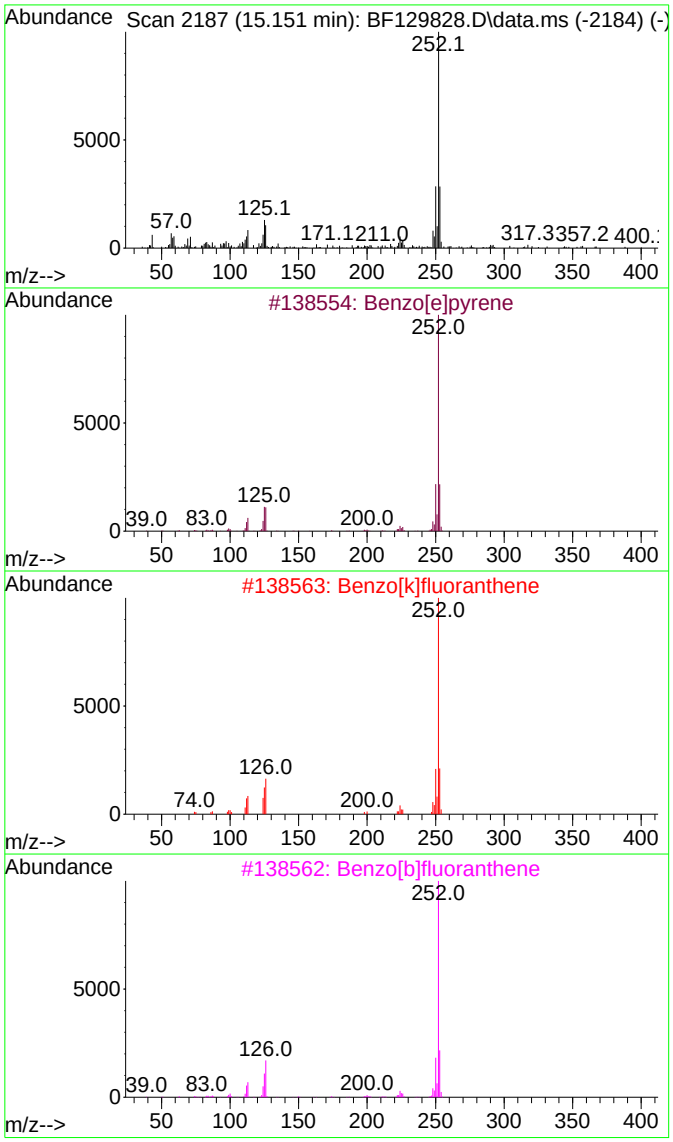
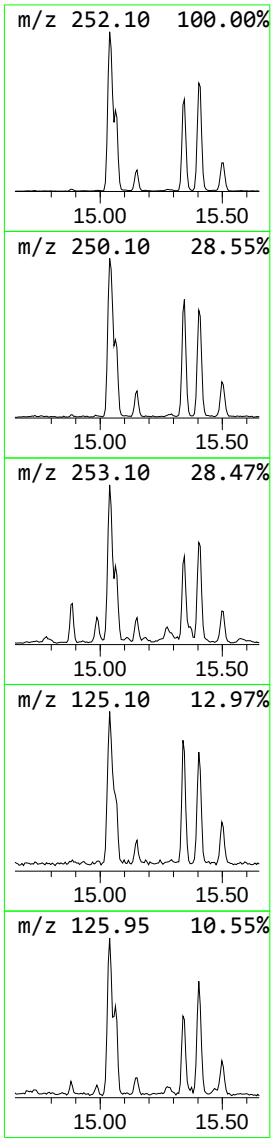
Peak Number 7 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.151	2.82 ng	112298	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	89
5	Perylene	252	C20H12	000198-55-0	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
Data File : BF129828.D
Acq On : 17 Aug 2022 00:33
Operator : CG\JU
Sample : N4191-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-367

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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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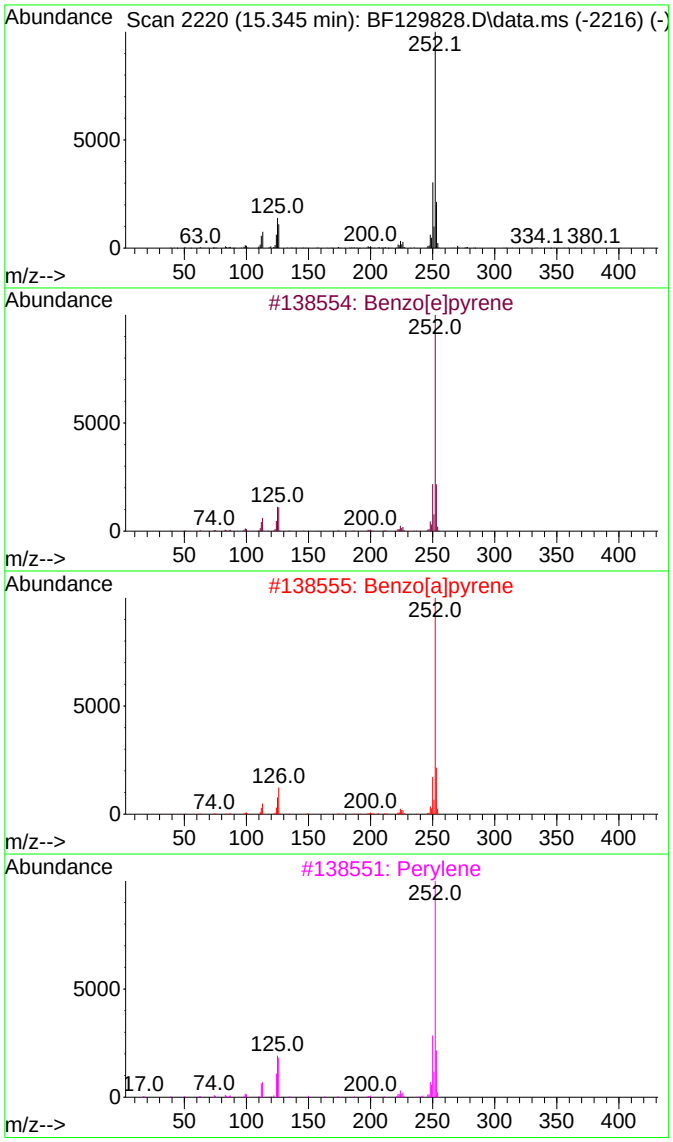
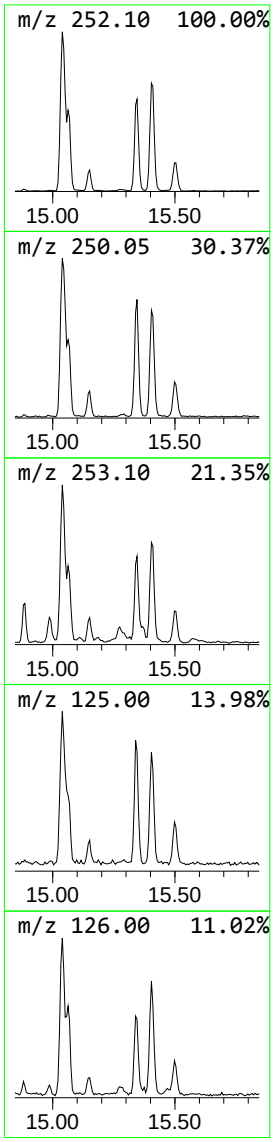
Peak Number 8 Perylene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.345	9.95 ng	396016	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[a]pyrene	252	C20H12	000050-32-8	96
3	Perylene	252	C20H12	000198-55-0	95
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
Data File : BF129828.D
Acq On : 17 Aug 2022 00:33
Operator : CG\JU
Sample : N4191-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-367

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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
3-Penten-2-one,...	4.416	4.0	ng	175113	1	6.822	871749	20.0
2-Pentanone, 4-...	5.046	10.6	ng	460567	1	6.822	871749	20.0
11H-Benzo[b]flu...	13.127	2.3	ng	144552	5	13.998	1236950	20.0
Cyclopenta[cd]p...	13.798	2.3	ng	140284	5	13.998	1236950	20.0
11H-Benzo[a]flu...	13.851	4.8	ng	297055	5	13.998	1236950	20.0
Phenanthrene, 1...	14.880	3.0	ng	120366	6	15.468	795769	20.0
Benzo[e]pyrene	15.151	2.8	ng	112298	6	15.468	795769	20.0
Perylene	15.345	9.9	ng	396016	6	15.468	795769	20.0