LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133281.D
Acq On : 06 May 2023 00:28
Operator : CG\JU
Sample : 02608-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-227

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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133281.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.922	477	482	495	rVB	669950	855143	19.76%	1.991%
2	5.345	549	554	557	rBV	4195005	4177336	96.50%	9.727%
3	6.369	723	728	731	rBV	4028163	4328665	100.00%	10.079%
4	6.722	785	788	792	rBV	1400859	1154435	26.67%	2.688%
5	7.292	880	885	888	rBV	3088960	2784763	64.33%	6.484%
6	8.010	1003	1007	1010	rBV	1920834	1555753	35.94%	3.623%
7	9.086	1185	1190	1193	rBV	4993065	4131017	95.43%	9.619%
8	9.345	1227	1234	1238	rBV2	38252	52152	1.20%	0.121%
9	9.416	1242	1246	1249	rBV	65838	66870	1.54%	0.156%
10	9.757	1301	1304	1307	rBV	2128465	1726415	39.88%	4.020%
11	9.786	1307	1309	1313	rVB	103770	89383	2.06%	0.208%
12	9.963	1335	1339	1343	rBV	106506	93383	2.16%	0.217%
13	10.304	1394	1397	1399	rBV	130180	107365	2.48%	0.250%
14	10.474	1421	1426	1429	rVB	612898	588040	13.58%	1.369%
15	10.551	1434	1439	1442	rBV	2929494	2944544	68.02%	6.856%
16	10.669	1455	1459	1466	rVB4	52653	60857	1.41%	0.142%
17	10.851	1484	1490	1493	rBV2	46306	55779	1.29%	0.130%
18	11.133	1536	1538	1547	rVB	81646	82032	1.90%	0.191%
19	11.239	1552	1556	1558	rVV	2088005	1744928	40.31%	4.063%
20	11.263	1558	1560	1563	rVV	1311928	967293	22.35%	2.252%
21	11.316	1563	1569	1572	rVB	217680	204814	4.73%	0.477%
22	11.568	1609	1612	1617	rVB	69229	63677	1.47%	0.148%
23	11.739	1637	1641	1644	rBV	219336	205324	4.74%	0.478%
24	11.780	1644	1648	1651	rVV2	611862	734913	16.98%	1.711%
25	11.816	1651	1654	1656	rVV2	103856	126288	2.92%	0.294%
26	11.851	1656	1660	1662	rVV2	289181	313781	7.25%	0.731%
27	11.874	1662	1664	1669	rVB	159350	136580	3.16%	0.318%
28	12.033	1688	1691	1693	rBV	85412	80358	1.86%	0.187%
29	12.057	1693	1695	1702	rVB2	101226	106567	2.46%	0.248%
30	12.215	1719	1722	1724	rBV	71095	55300	1.28%	0.129%
31	12.292	1731	1735	1738	rBV	171467	182764	4.22%	0.426%
32	12.321	1738	1740	1743	rVV2	79332	100625	2.32%	0.234%
33	12.374	1746	1749	1753	rVV2	85444	96416	2.23%	0.225%
34	12.451	1758	1762	1765	rBV	1370525	1118157	25.83%	2.604%
35	12.563	1777	1781	1785	rBV4	99656	142047	3.28%	0.331%
36	12.598	1785	1787	1791	rVV2	54332	66890	1.55%	0.156%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133281.D
Acq On : 06 May 2023 00:28
Operator : CG\JU
Sample : 02608-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-227

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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.674	1795	1800	1803	rVV	1094672	1118365	25.84%	2.604%
38	12.739	1807	1811	1814	rVB3	67826	97791	2.26%	0.228%
39	12.798	1817	1821	1822	rBV2	54605	49239	1.14%	0.115%
40	12.827	1822	1826	1829	rVV	3805965	3406511	78.70%	7.932%
41	12.898	1833	1838	1841	rBV2	91090	132957	3.07%	0.310%
42	12.986	1849	1853	1854	rBV2	65225	76722	1.77%	0.179%
43	13.004	1854	1856	1860	rVB2	121988	117097	2.71%	0.273%
44	13.068	1860	1867	1870	rBV2	87405	131052	3.03%	0.305%
45	13.110	1870	1874	1877	rBV2	151922	149790	3.46%	0.349%
46	13.198	1886	1889	1892	rBV	89184	82302	1.90%	0.192%
47	13.233	1892	1895	1899	rVB	84592	76465	1.77%	0.178%
48	13.510	1939	1942	1947	rVB	87372	88224	2.04%	0.205%
49	13.621	1956	1961	1964	rBV3	92632	140539	3.25%	0.327%
50	13.727	1975	1979	1987	rBV4	300378	450332	10.40%	1.049%
51	13.874	1999	2004	2006	rBV2	1457594	1557923	35.99%	3.628%
52	13.898	2006	2008	2014	rVB	354048	305534	7.06%	0.711%
53	13.968	2014	2020	2026	rBV	990110	1130380	26.11%	2.632%
54	14.051	2032	2034	2038	rVB3	56347	52250	1.21%	0.122%
55	14.257	2066	2069	2073	rVB	84848	92884	2.15%	0.216%
56	14.357	2083	2086	2088	rBV2	66060	58872	1.36%	0.137%
57	14.651	2134	2136	2144	rVB2	57893	80172	1.85%	0.187%
58	14.886	2172	2176	2183	rBV	250567	432404	9.99%	1.007%
59	14.986	2188	2193	2198	rVB2	57341	104234	2.41%	0.243%
60	15.168	2221	2224	2231	rVB	132889	164066	3.79%	0.382%
61	15.227	2231	2234	2240	rVB	192455	216425	5.00%	0.504%
62	15.292	2240	2245	2248	rBV	890631	1008822	23.31%	2.349%
63	15.745	2318	2322	2326	rBV	46560	65313	1.51%	0.152%
64	16.656	2473	2477	2483	rVB3	74651	138666	3.20%	0.323%
65	17.068	2543	2547	2556	rVB	62257	119327	2.76%	0.278%

Sum of corrected areas: 42945312

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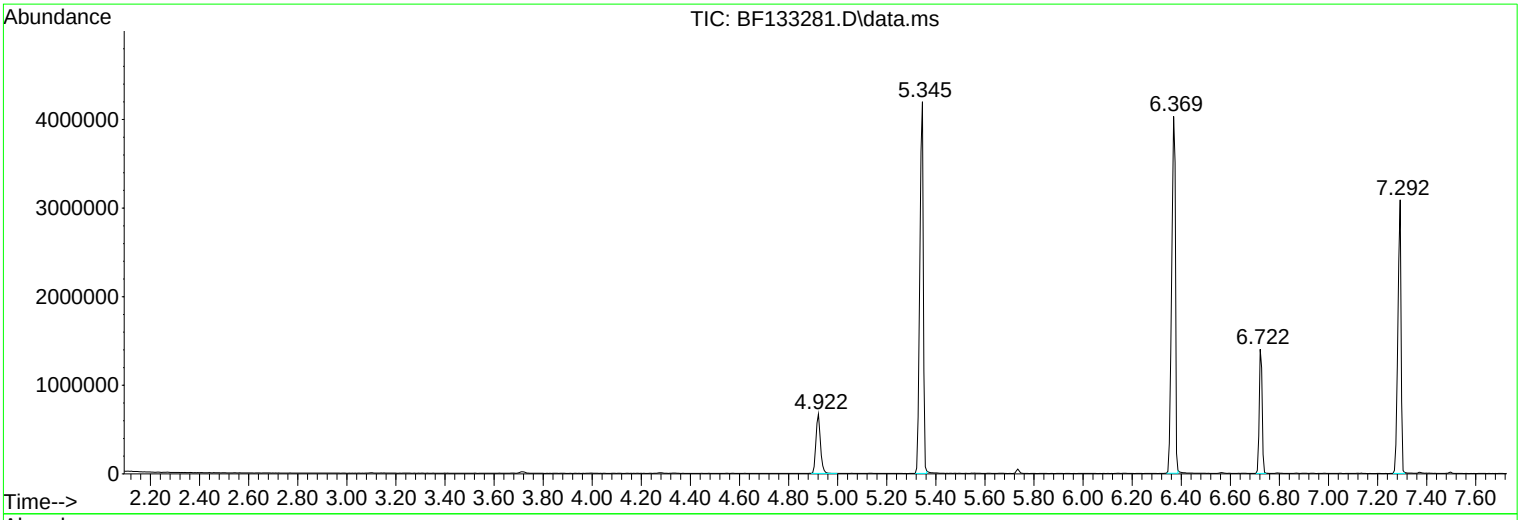
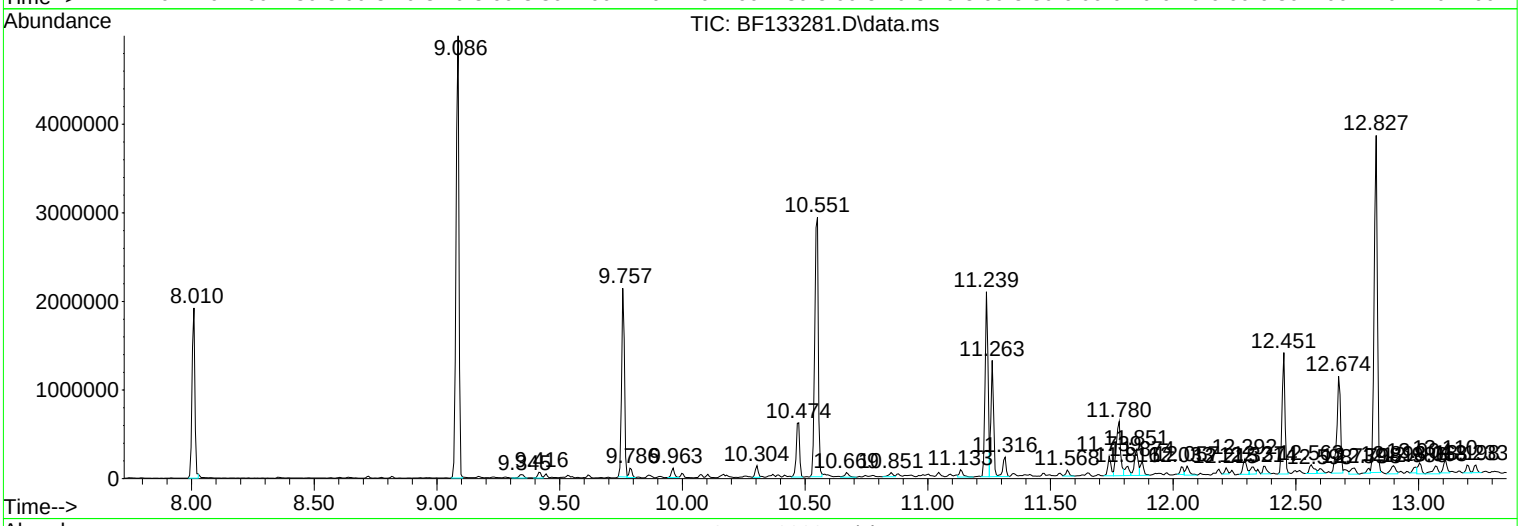
Misc :
ALS Vial : 18 Sample Multiplier: 1

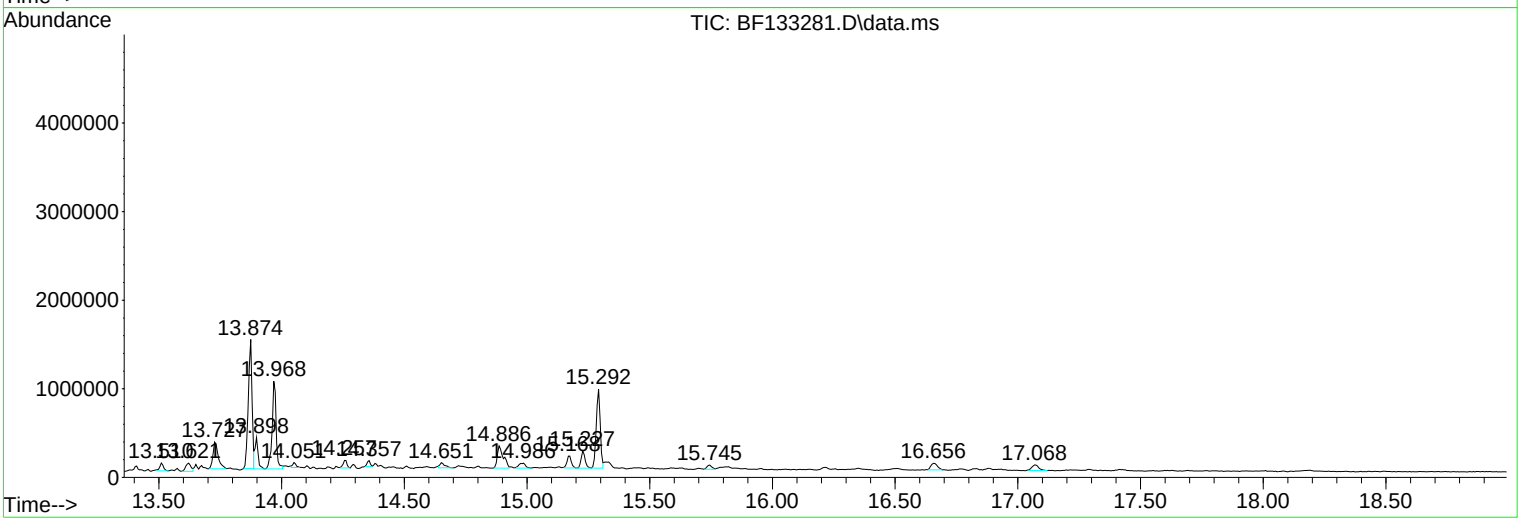
Instrument :
BNA_F
ClientSampleId :
VNJ-227

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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Sample : 02608-01
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Instrument :
BNA_F
ClientSampleId :
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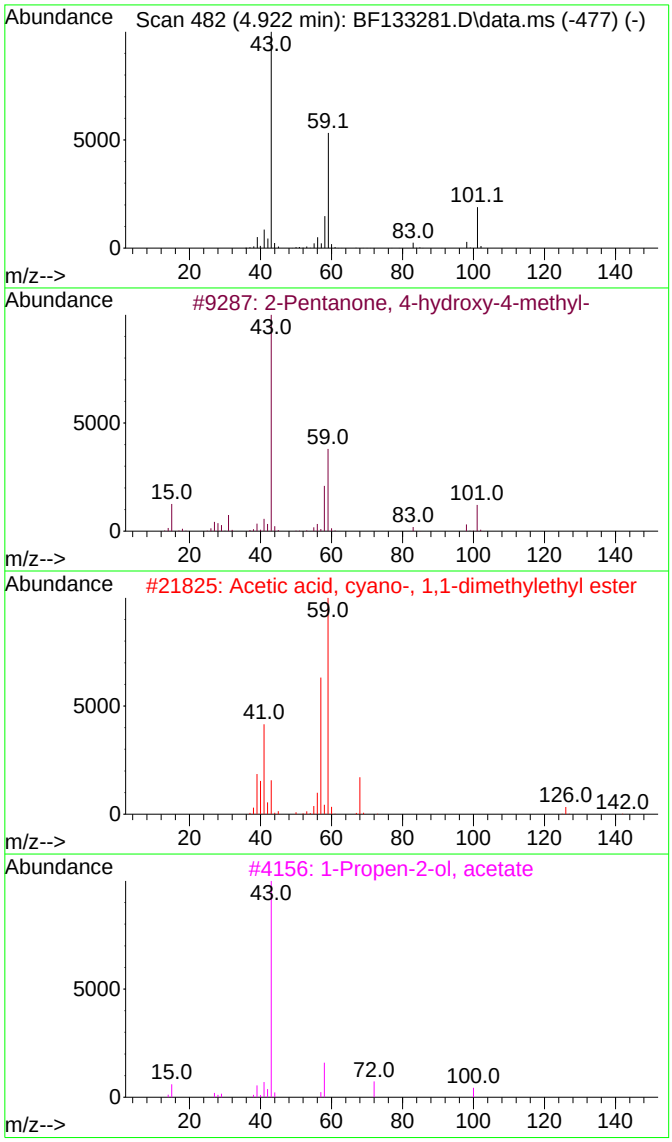
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

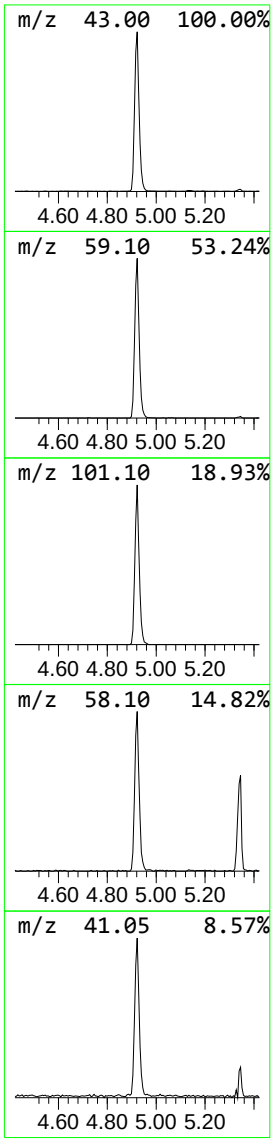
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.922	14.81 ng	855143	1,4-Dichlorobenzene-d4	6.722

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9





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Operator : CG\JU
Sample : 02608-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-227

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

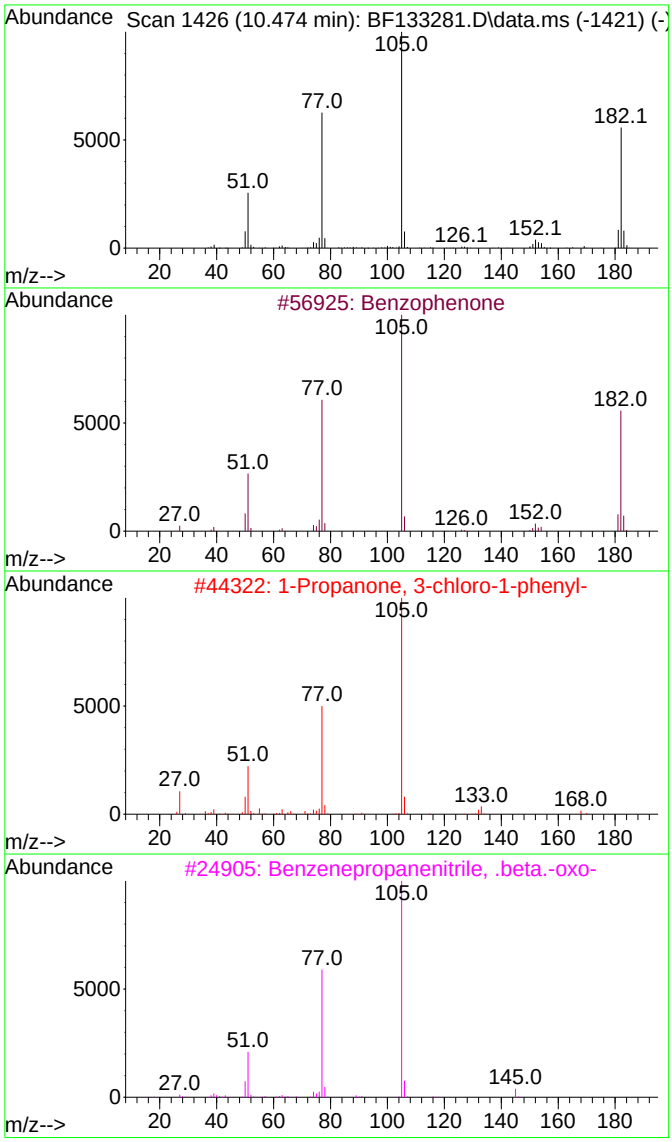
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

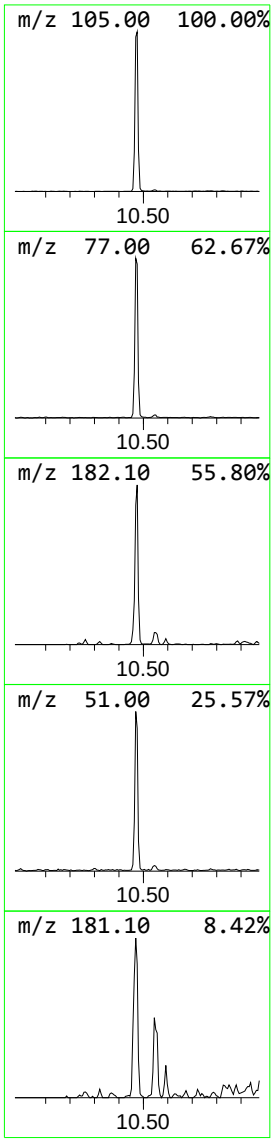
****

Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.474	6.81 ng	588040	Acenaphthene-d10	9.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
3	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
4	N-Methylbenzamide, N-heptafluoro...	331	C12H8F7NO2	1000446-97-2	47
5	Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	47





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Sample : 02608-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-227

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

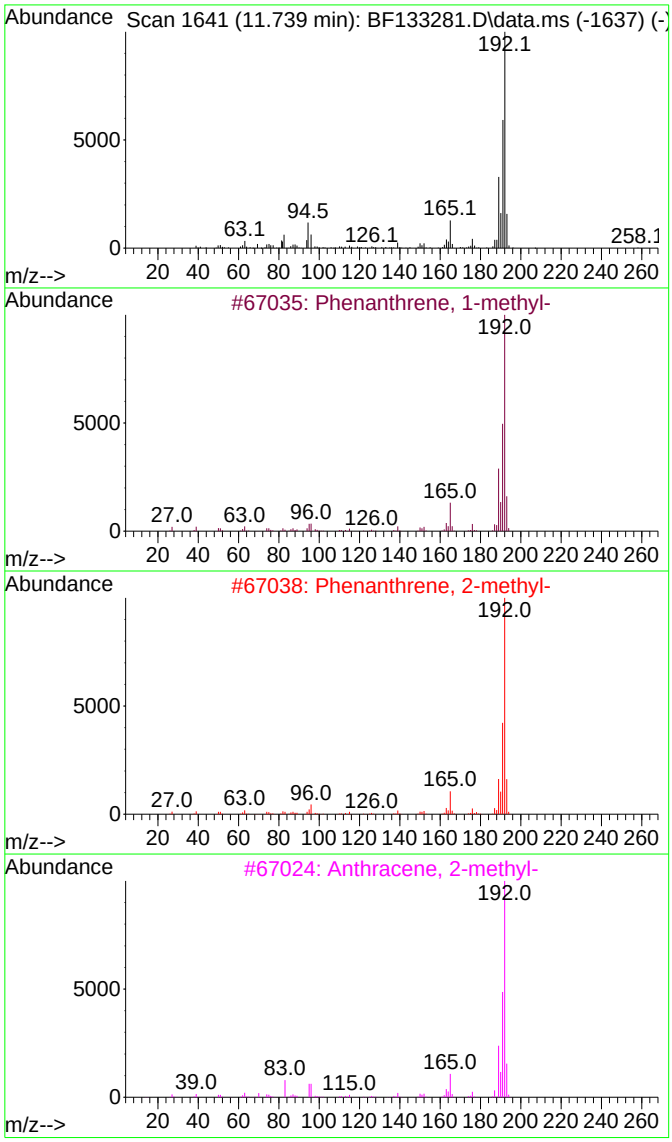
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

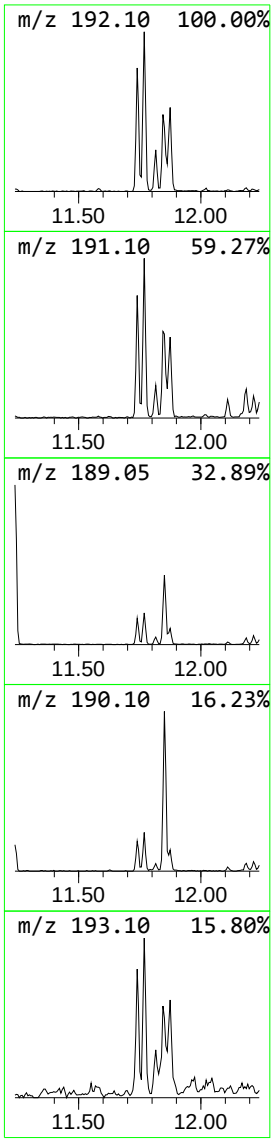
****

Peak Number 4 Phenanthrene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.739	2.35 ng	205324	Phenanthrene-d10	11.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	97
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
4	1H-Indene, 1-phenyl-	192	C15H12	001961-96-2	94
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	94





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

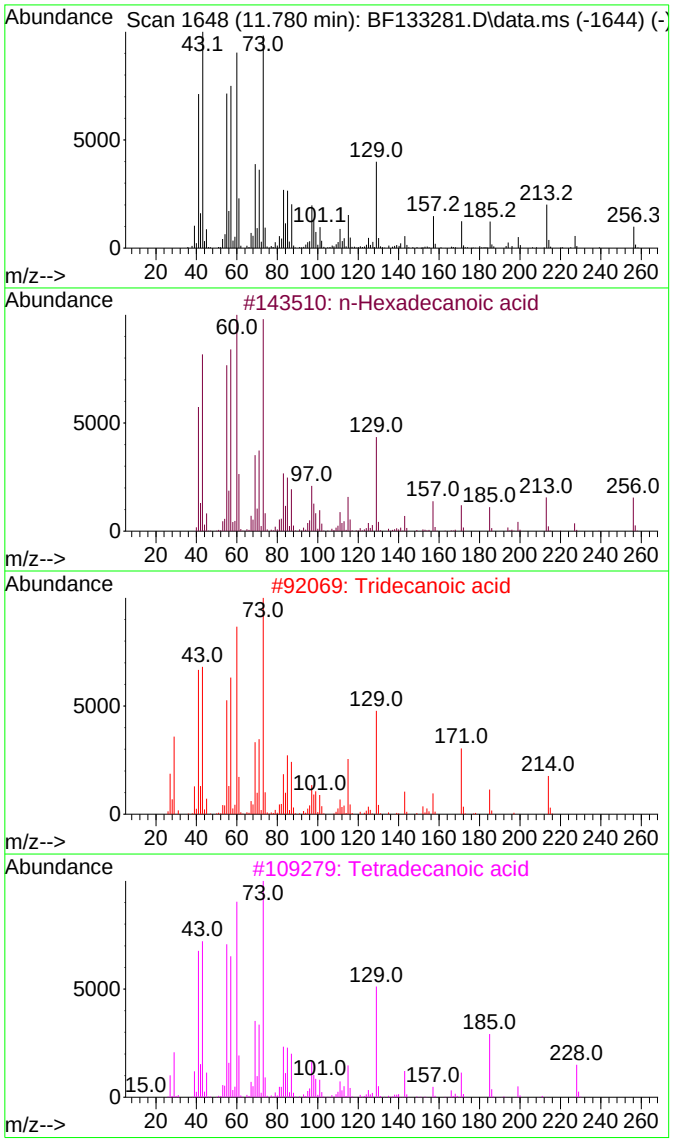
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

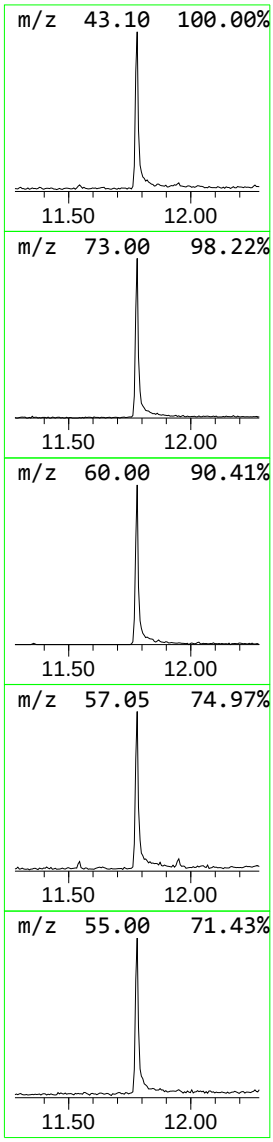
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.780	8.42 ng	734913	Phenanthrene-d10	11.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





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BNA_F
ClientSampleId :
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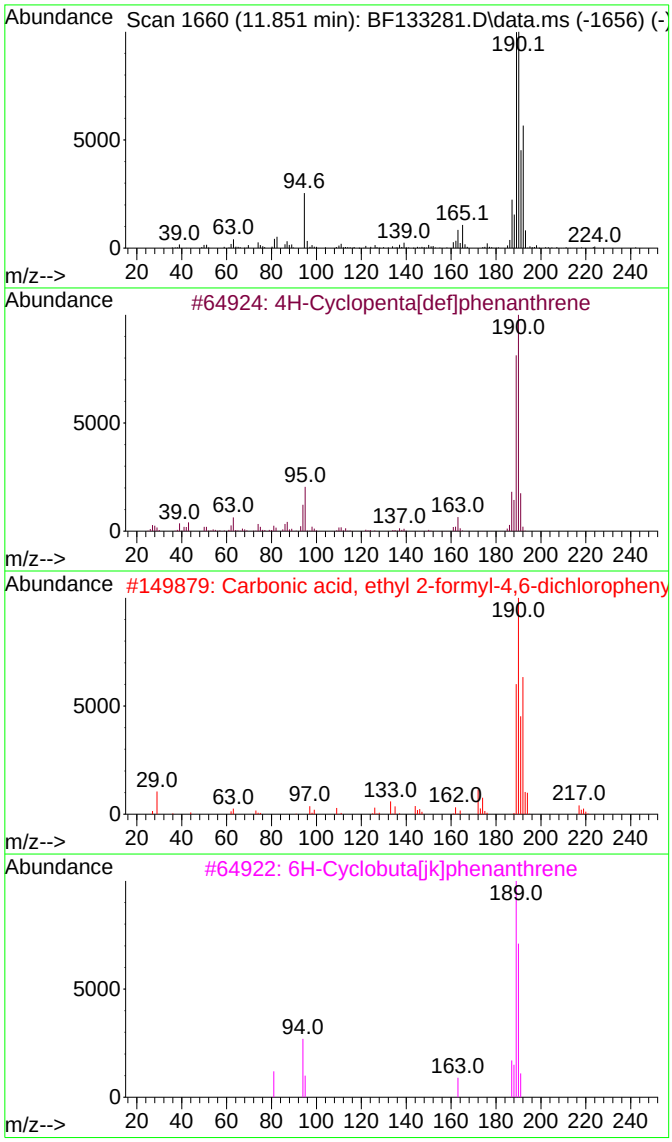
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

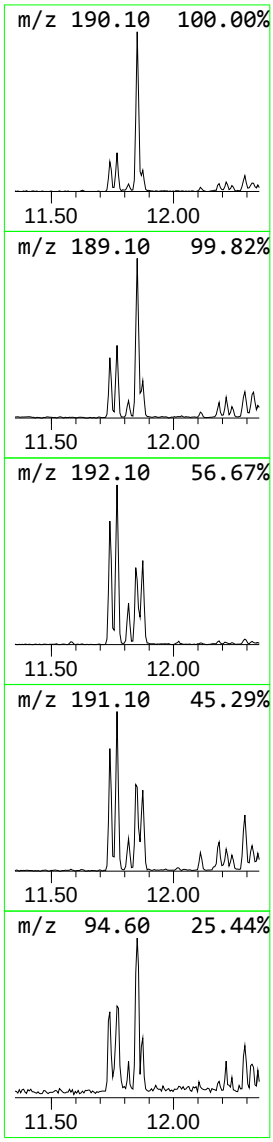
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	3.60 ng	313781	Phenanthrene-d10	11.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	50
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	40
4	2-Amino-4,6-dichloropyrimidine-5...	191	C5H3Cl2N3O	005604-46-6	38
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	20





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Data File : BF133281.D
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Operator : CG\JU
Sample : 02608-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-227

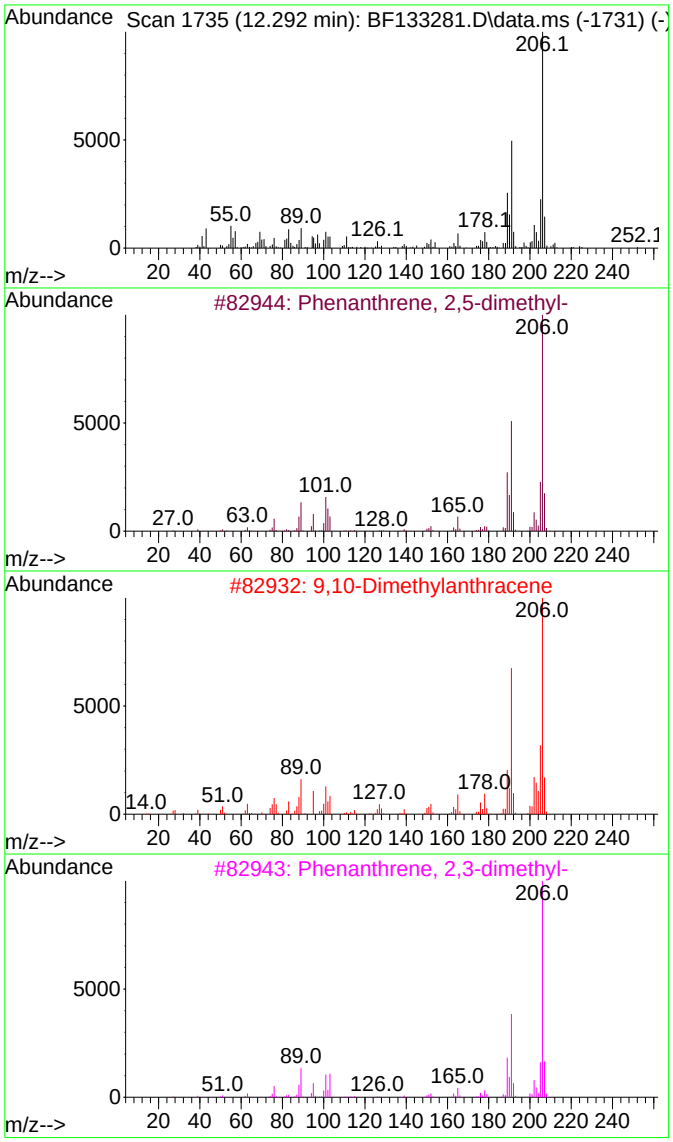
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

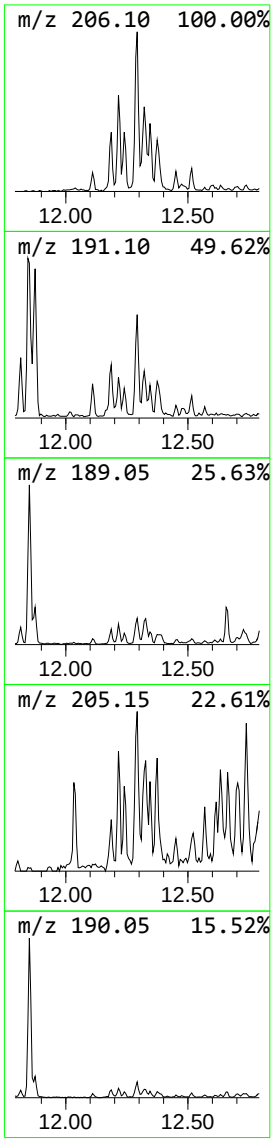
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Phenanthrene, 2,5-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.292	2.09 ng	182764	Phenanthrene-d10	11.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	97
2	9,10-Dimethylanthracene	206	C16H14	000781-43-1	93
3	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	90
4	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	90
5	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133281.D
Acq On : 06 May 2023 00:28
Operator : CG\JU
Sample : 02608-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-227

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

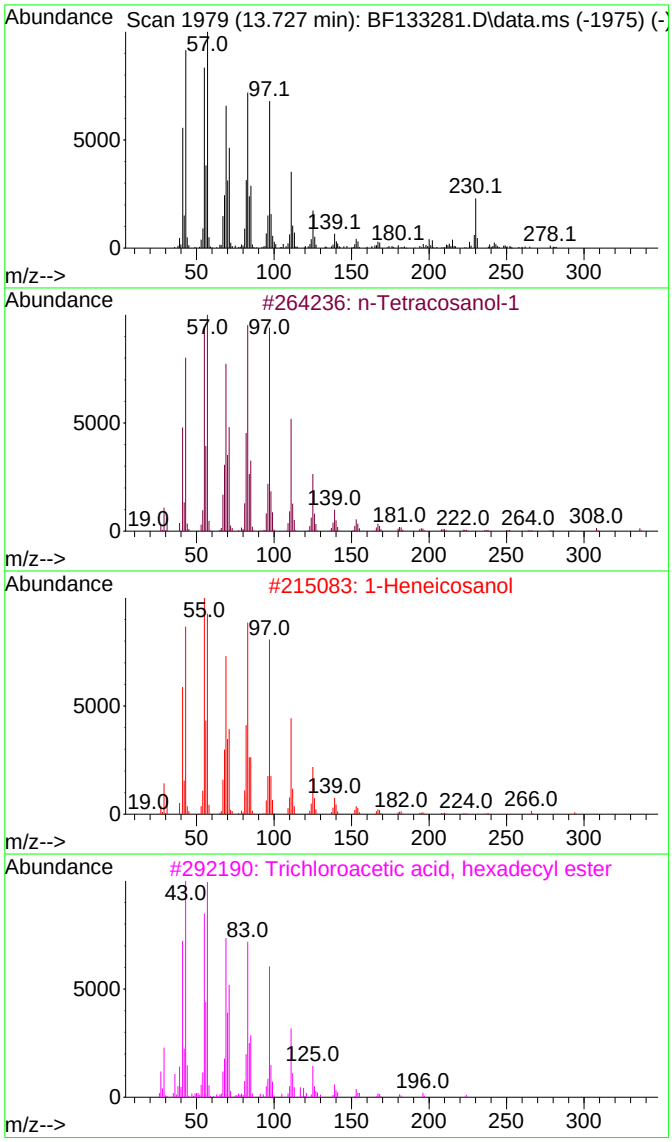
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

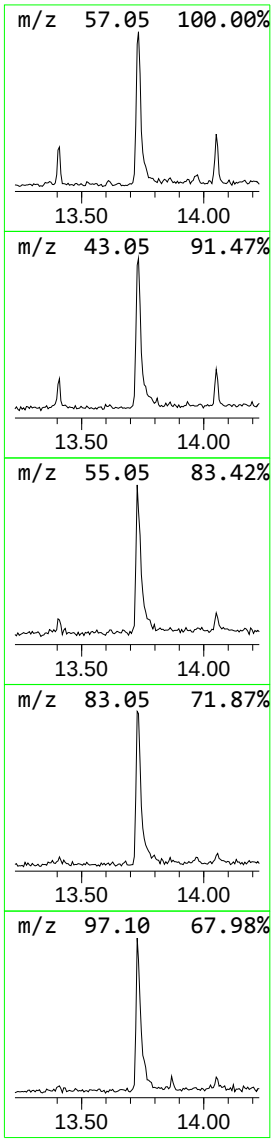
****

Peak Number 8 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.727	5.78 ng	450332	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
5	Behenic alcohol	326	C22H46O	000661-19-8	91





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Data File : BF133281.D
Acq On : 06 May 2023 00:28
Operator : CG\JU
Sample : 02608-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-227

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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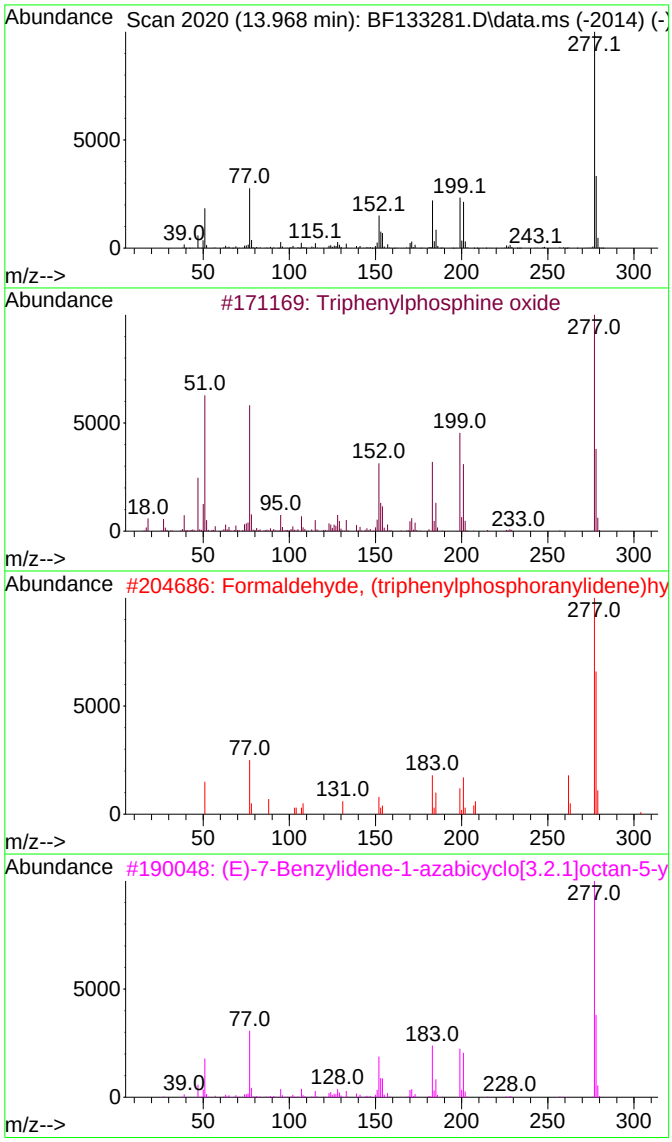
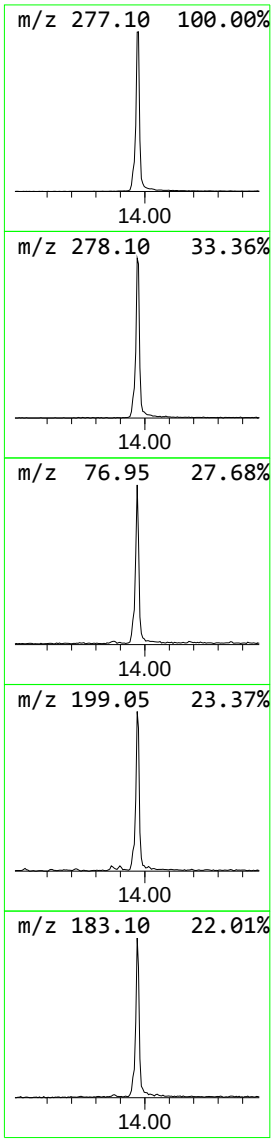
Peak Number 9 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.968	14.51 ng	1130380	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
3	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	64
4	4-Nitro-4'-methyldiphenylsulfone	277	C13H11NO4S	004094-37-5	43
5	2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133281.D
Acq On : 06 May 2023 00:28
Operator : CG\JU
Sample : 02608-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-227

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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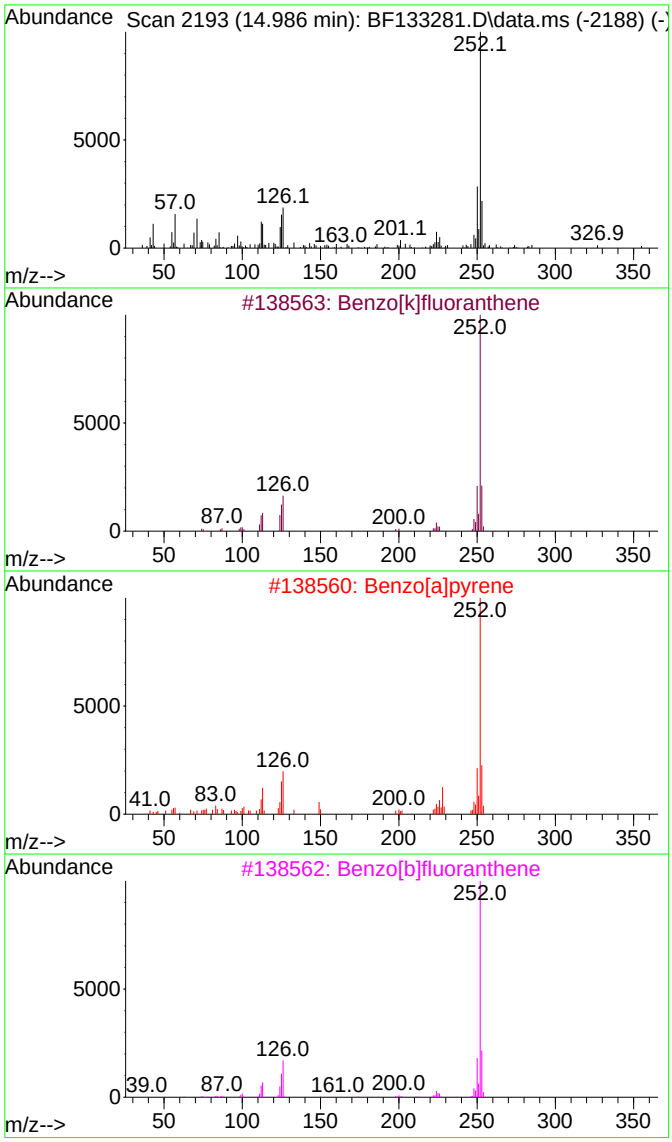
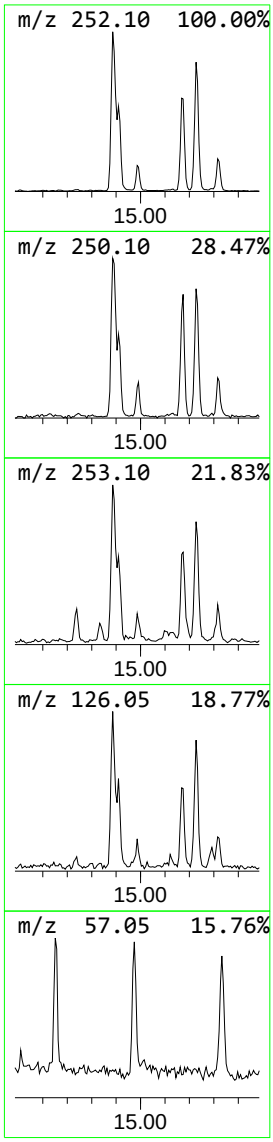
Peak Number 10 Perylene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.986	2.07 ng	104234	Perylene-d12	15.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
2	Benzo[a]pyrene	252	C20H12	000050-32-8	93
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	91
4	Perylene	252	C20H12	000198-55-0	90
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	89





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133281.D
Acq On : 06 May 2023 00:28
Operator : CG\JU
Sample : 02608-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-227

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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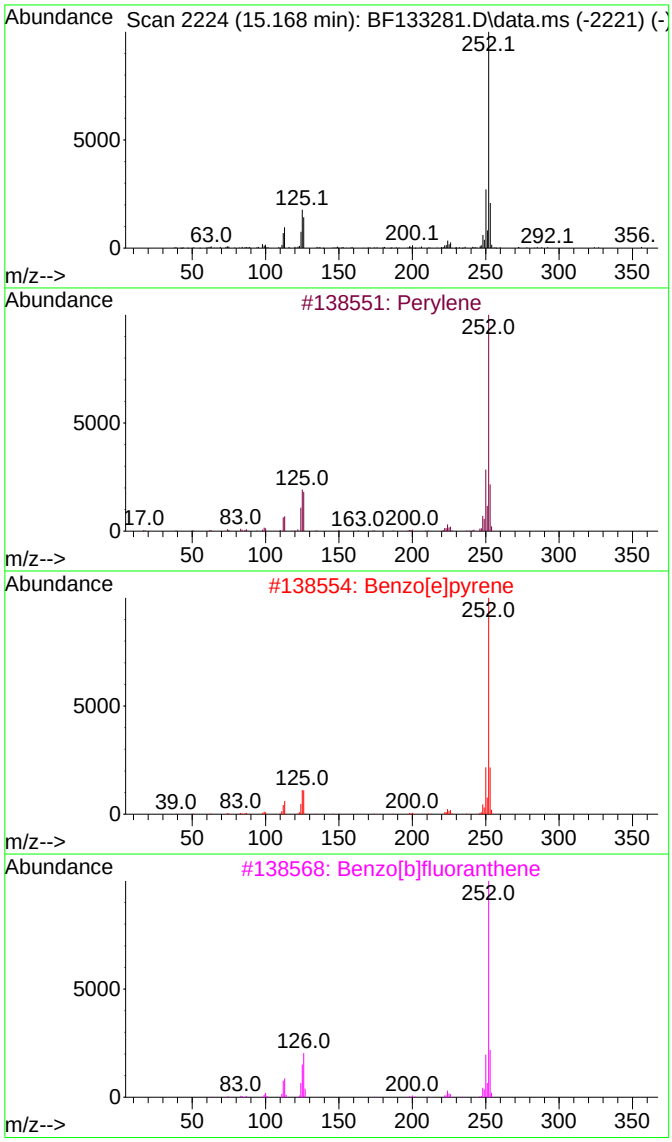
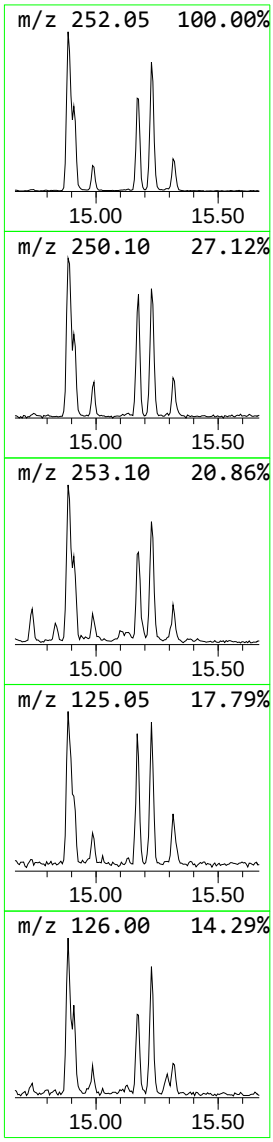
Peak Number 11 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.168	3.25 ng	164066	Perylene-d12	15.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	99
2	Benzo[e]pyrene	252	C20H12	000192-97-2	98
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
4	Benzo[a]pyrene	252	C20H12	000050-32-8	94
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133281.D
Acq On : 06 May 2023 00:28
Operator : CG\JU
Sample : 02608-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-227

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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-...	4.922	14.8	ng	855143	1	6.722	1154440	20.0
Benzophenone	10.474	6.8	ng	588040	3	9.757	1726420	20.0
Phenanthrene, 1...	11.739	2.4	ng	205324	4	11.239	1744930	20.0
n-Hexadecanoic ...	11.780	8.4	ng	734913	4	11.239	1744930	20.0
4H-Cyclopenta[d...	11.851	3.6	ng	313781	4	11.239	1744930	20.0
Phenanthrene, 2...	12.292	2.1	ng	182764	4	11.239	1744930	20.0
n-Tetracosanol-1	13.727	5.8	ng	450332	5	13.874	1557920	20.0
Triphenylphosph...	13.968	14.5	ng	1130380	5	13.874	1557920	20.0
Perylene	14.986	2.1	ng	104234	6	15.292	1008820	20.0
Benzo[e]pyrene	15.168	3.3	ng	164066	6	15.292	1008820	20.0