LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
Data File : BF134405.D
Acq On : 21 Jul 2023 17:19
Operator : CG\JU
Sample : 03640-21
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP12

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134405.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.151	3	11	24	rVB	187060	264347	15.50%	1.857%
2	5.098	508	512	522	rBV	18675	27229	1.60%	0.191%
3	5.481	573	577	595	rBV	1546328	1447360	84.86%	10.166%
4	6.481	742	747	750	rBV	1531948	1418511	83.17%	9.963%
5	6.534	754	756	767	rVB2	25228	30065	1.76%	0.211%
6	6.833	804	807	813	rBV	405583	358156	21.00%	2.516%
7	7.404	899	904	907	rBV	1038821	943659	55.33%	6.628%
8	7.857	978	981	985	rBV	77496	58076	3.41%	0.408%
9	8.116	1021	1025	1028	rBV	583407	456062	26.74%	3.203%
10	9.192	1204	1208	1211	rBV	2212828	1705575	100.00%	11.979%
11	9.522	1261	1264	1269	rVB3	24359	21085	1.24%	0.148%
12	9.874	1320	1324	1327	rBV	576248	497753	29.18%	3.496%
13	10.669	1455	1459	1475	rVB	1385625	1161160	68.08%	8.155%
14	11.369	1574	1578	1580	rBV	626057	501271	29.39%	3.521%
15	11.392	1580	1582	1586	rVV	177653	138637	8.13%	0.974%
16	11.445	1588	1591	1594	rVB	31190	26500	1.55%	0.186%
17	11.868	1659	1663	1666	rBV2	47686	67510	3.96%	0.474%
18	11.898	1666	1668	1673	rVB2	225786	194415	11.40%	1.365%
19	11.986	1680	1683	1685	rBV2	52406	54522	3.20%	0.383%
20	12.010	1685	1687	1690	rVB	25097	21806	1.28%	0.153%
21	12.427	1754	1758	1760	rBV	23582	25855	1.52%	0.182%
22	12.463	1760	1764	1767	rVV4	21143	26250	1.54%	0.184%
23	12.515	1770	1773	1778	rBV2	26543	29772	1.75%	0.209%
24	12.592	1782	1786	1789	rBV	438736	369469	21.66%	2.595%
25	12.692	1799	1803	1808	rBV2	29760	40854	2.40%	0.287%
26	12.821	1819	1825	1831	rBV	373392	372328	21.83%	2.615%
27	12.968	1841	1850	1853	rBV	1477962	1383387	81.11%	9.716%
28	13.039	1858	1862	1868	rBV3	24486	41460	2.43%	0.291%
29	13.127	1874	1877	1879	rBV3	21620	26804	1.57%	0.188%
30	13.151	1879	1881	1885	rVB	40139	41958	2.46%	0.295%
31	13.257	1896	1899	1907	rVB2	38901	49631	2.91%	0.349%
32	13.351	1911	1915	1917	rBV	24328	21380	1.25%	0.150%
33	13.668	1966	1969	1973	rVB	32383	32168	1.89%	0.226%
34	13.780	1985	1988	1990	rBV2	30320	28322	1.66%	0.199%
35	13.880	2001	2005	2008	rBV2	32582	39499	2.32%	0.277%
36	13.933	2008	2014	2015	rBV5	53896	92049	5.40%	0.647%

LSC Area Percent Report

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Acq On : 21 Jul 2023 17:19
Operator : CG\JU
Sample : 03640-21
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP12

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.033	2026	2031	2033	rBV2	409523	507215	29.74%	3.562%
38	14.057	2033	2035	2038	rVB	171100	130390	7.64%	0.916%
39	14.186	2054	2057	2059	rBV2	28325	32572	1.91%	0.229%
40	14.421	2095	2097	2100	rVB	37775	30542	1.79%	0.215%
41	14.457	2101	2103	2107	rVB3	21989	21680	1.27%	0.152%
42	14.498	2107	2110	2113	rBV3	25092	30099	1.76%	0.211%
43	14.927	2180	2183	2186	rBV3	17755	24987	1.47%	0.175%
44	14.962	2186	2189	2192	rVB2	37431	41147	2.41%	0.289%
45	15.092	2207	2211	2214	rBV	166130	235861	13.83%	1.657%
46	15.157	2220	2222	2227	rVB4	26896	33094	1.94%	0.232%
47	15.204	2227	2230	2235	rVB	27914	33333	1.95%	0.234%
48	15.409	2260	2265	2269	rBV	90648	136416	8.00%	0.958%
49	15.474	2272	2276	2281	rVB	164059	233949	13.72%	1.643%
50	15.539	2282	2287	2291	rBV	287287	364237	21.36%	2.558%
51	16.009	2365	2367	2373	rVB4	25047	34067	2.00%	0.239%
52	17.086	2544	2550	2558	rVB3	53804	129945	7.62%	0.913%
53	17.174	2561	2565	2572	rVB9	17905	34819	2.04%	0.245%
54	17.274	2578	2582	2587	rVB7	12607	23979	1.41%	0.168%
55	17.550	2624	2629	2641	rVB4	36805	88408	5.18%	0.621%
56	17.821	2666	2675	2678	rBV8	21587	56223	3.30%	0.395%

Sum of corrected areas: 14237848

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
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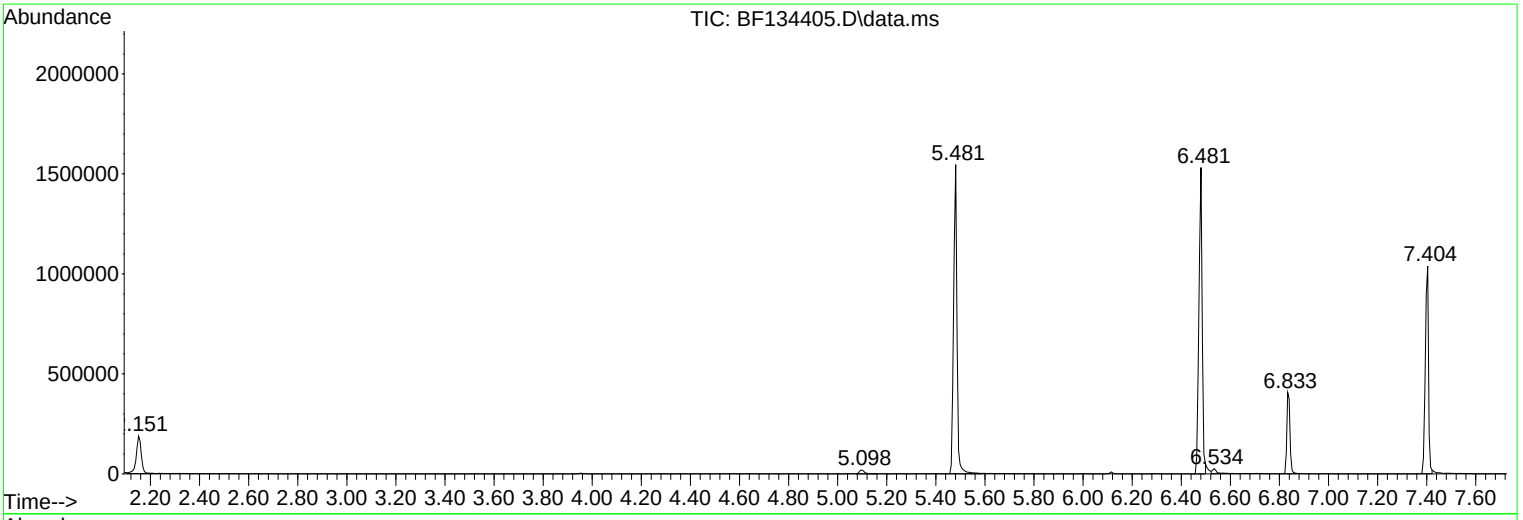
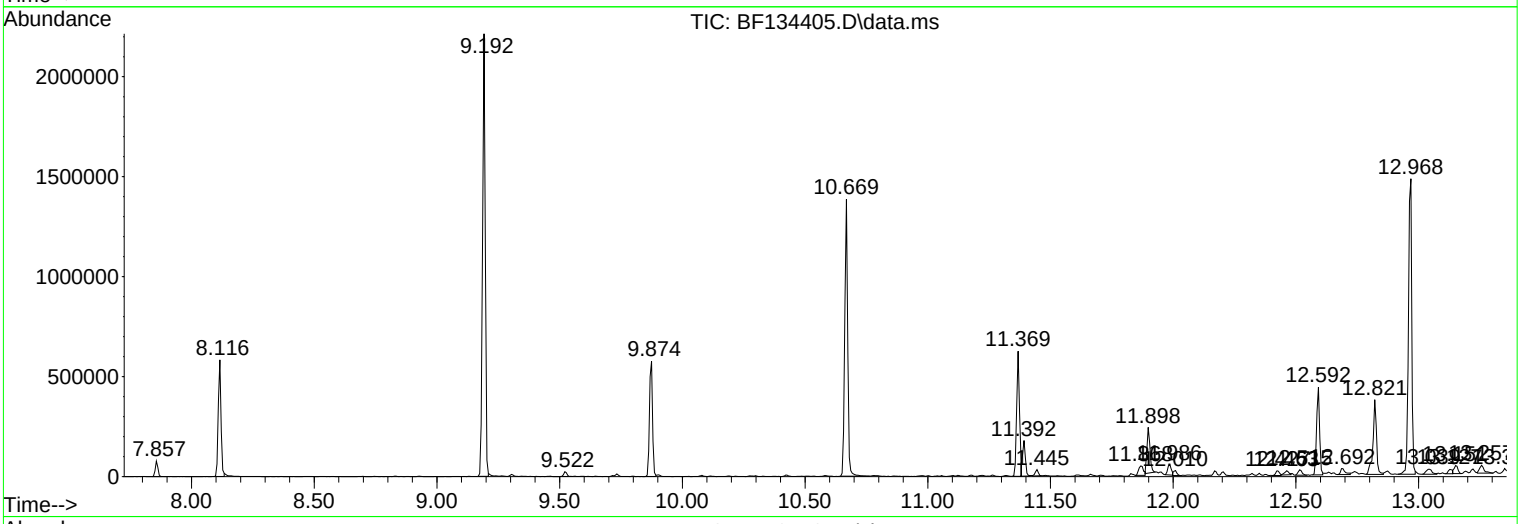
Sample : 03640-21
Misc :
ALS Vial : 15 Sample Multiplier: 1

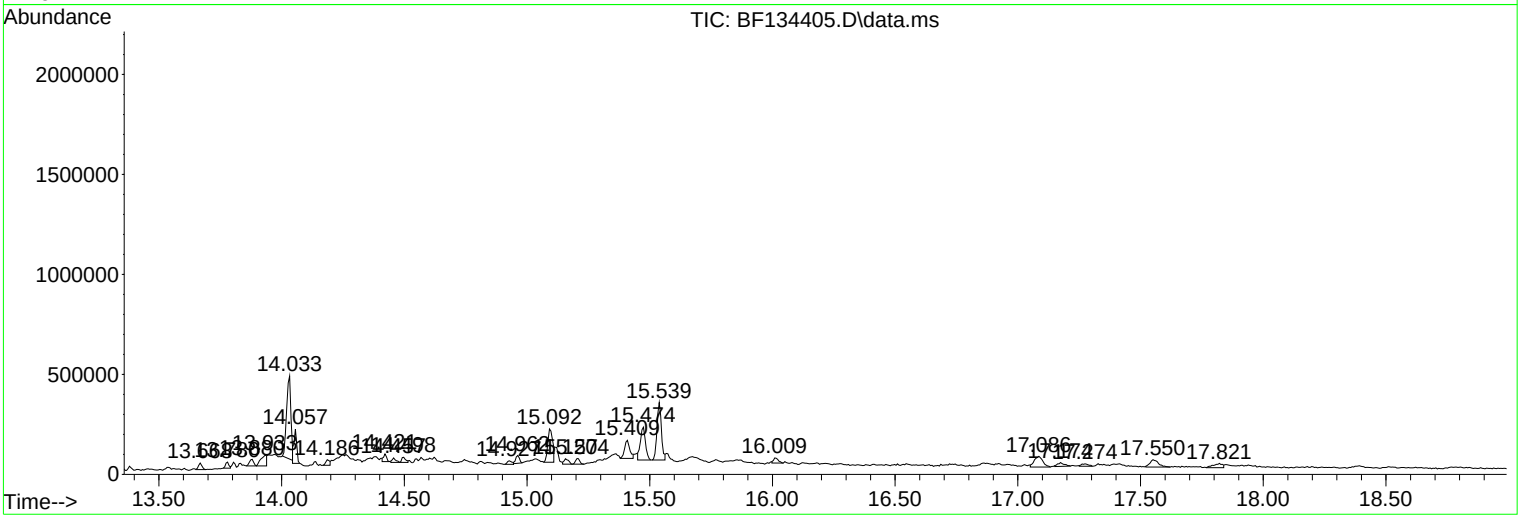
Instrument :
BNA_F
ClientSampleId :
TP12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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\BF072123\
Data File : BF134405.D
Acq On : 21 Jul 2023 17:19
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Sample : 03640-21
Misc :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

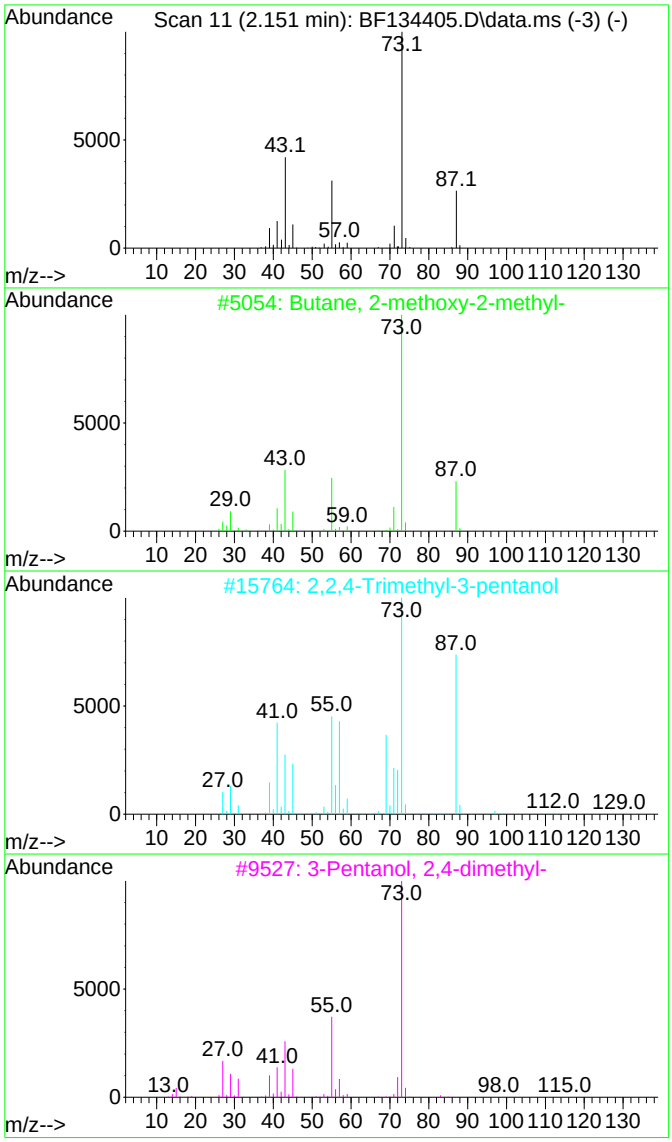
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

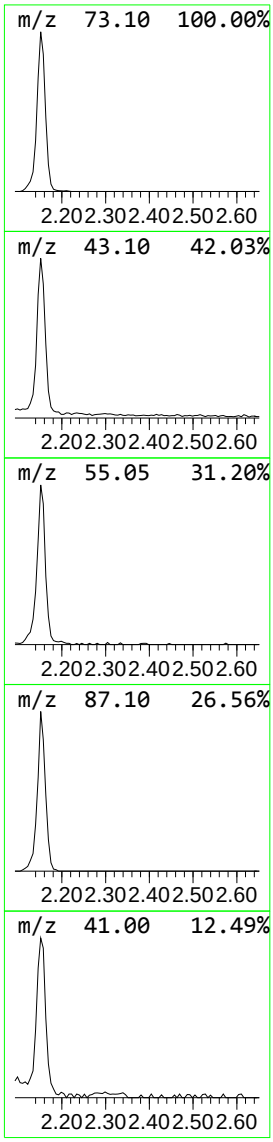
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.151	14.76 ng	264347	1,4-Dichlorobenzene-d4	6.839

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	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
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\BF072123\
Data File : BF134405.D
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Operator : CG\JU
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Instrument :
BNA_F
ClientSampleId :
TP12

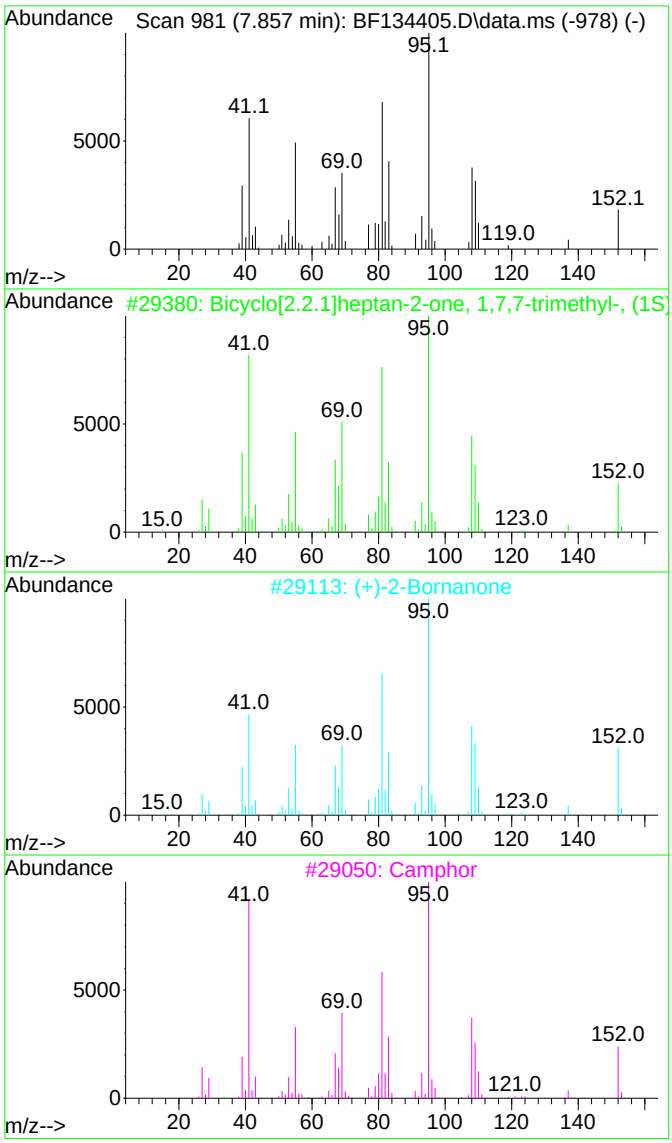
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

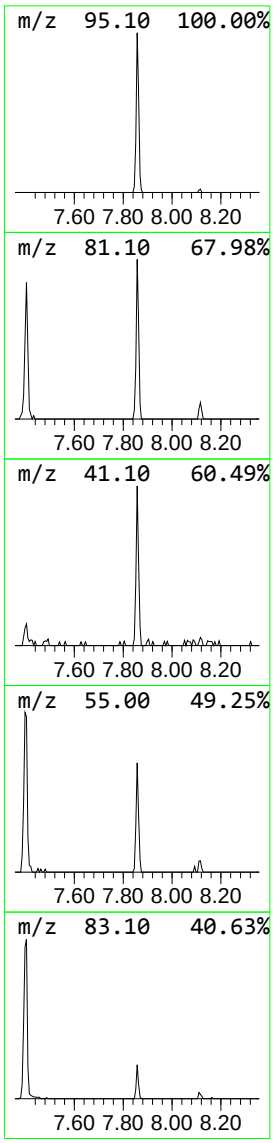
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.857	2.55 ng	58076	Naphthalene-d8	8.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	97
2	(+)-2-Bornanone	152	C10H16O	000464-49-3	96
3	Camphor	152	C10H16O	000076-22-2	93
4	Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1010142-17-5	46
5	5-Hepten-2-ol, 6-methyl-	128	C8H16O	001569-60-4	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
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Sample : 03640-21
Misc :
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

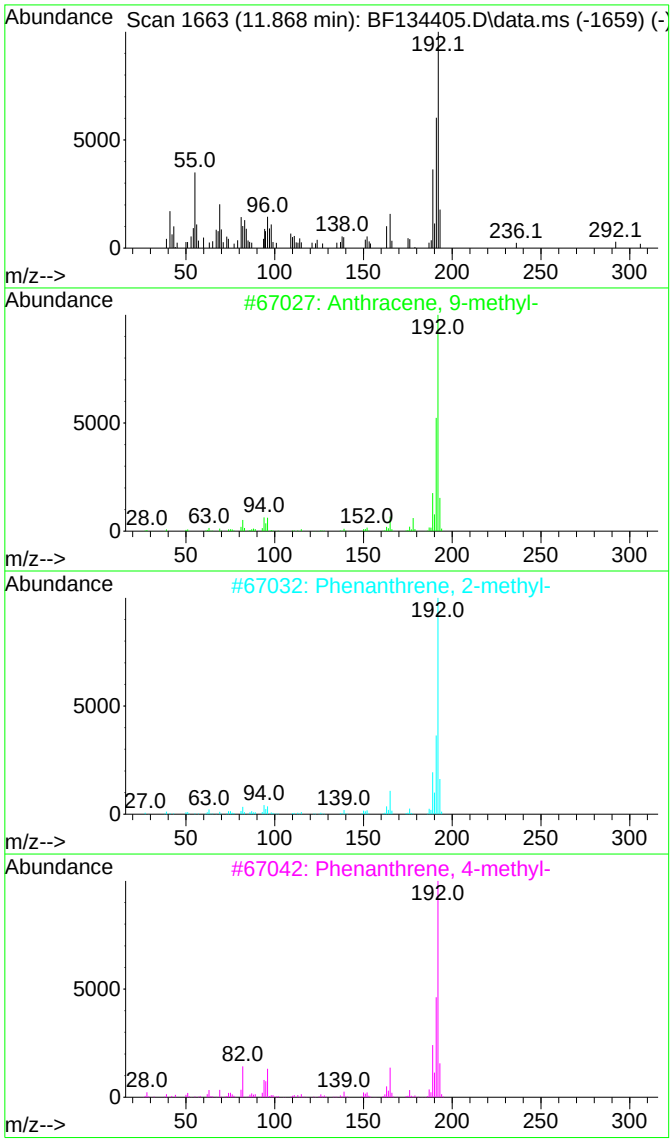
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

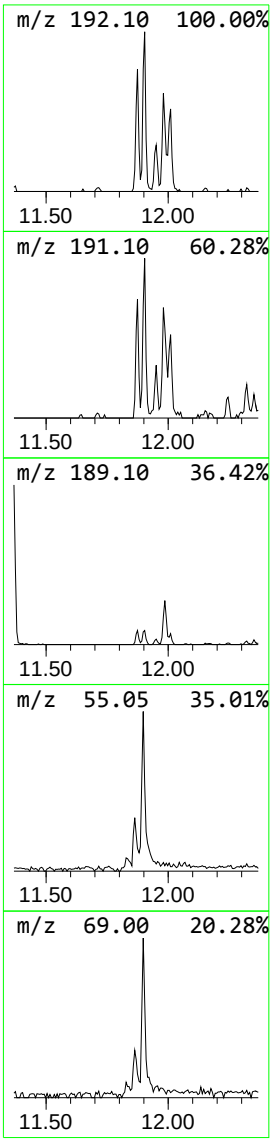
****

Peak Number 3 Anthracene, 9-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.868	2.69 ng	67510	Phenanthrene-d10	11.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 9-methyl-	192	C15H12	000779-02-2	94
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	90
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	81
5	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
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Acq On : 21 Jul 2023 17:19
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Sample : 03640-21
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

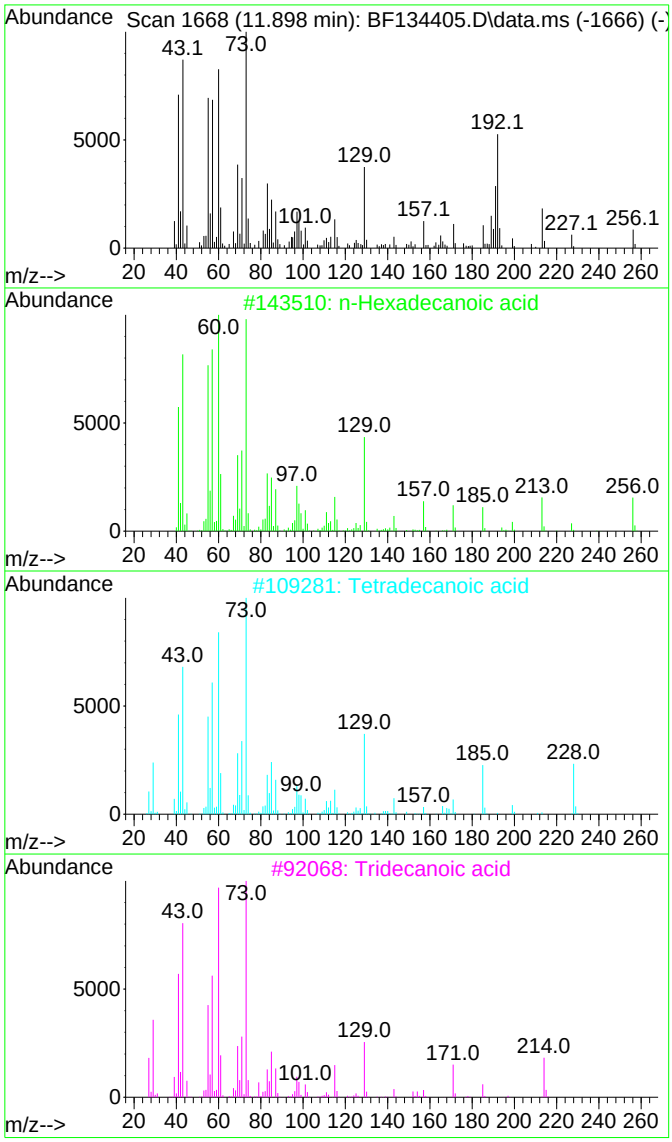
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

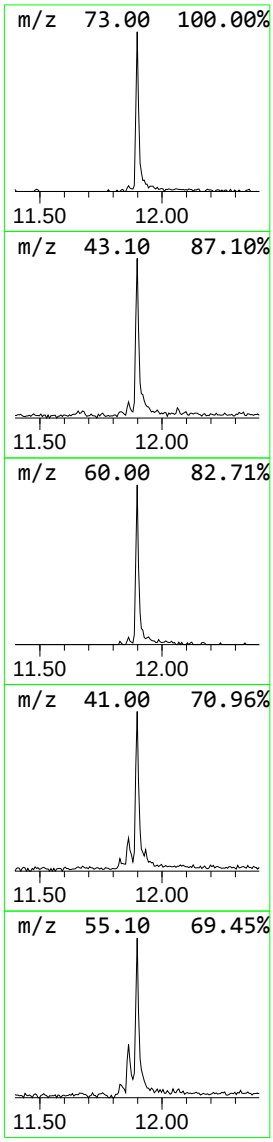
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	7.76 ng	194415	Phenanthrene-d10	11.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	78
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	68
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
Data File : BF134405.D
Acq On : 21 Jul 2023 17:19
Operator : CG\JU
Sample : 03640-21
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

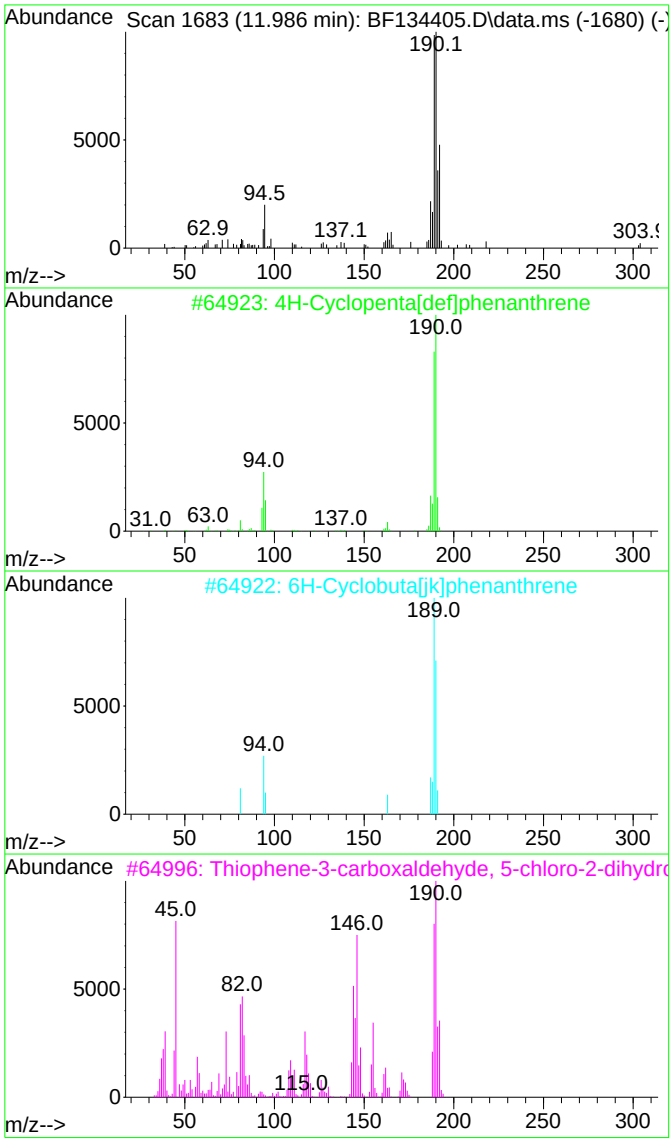
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

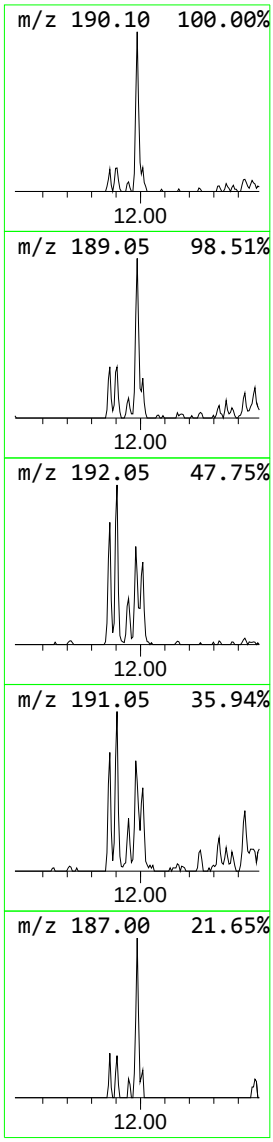
****

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.986	2.18 ng	54522	Phenanthrene-d10	11.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	59
3	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	50
4	Methyl diselenide	190	C2H6Se2	007101-31-7	46
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38





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Data File : BF134405.D
Acq On : 21 Jul 2023 17:19
Operator : CG\JU
Sample : 03640-21
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP12

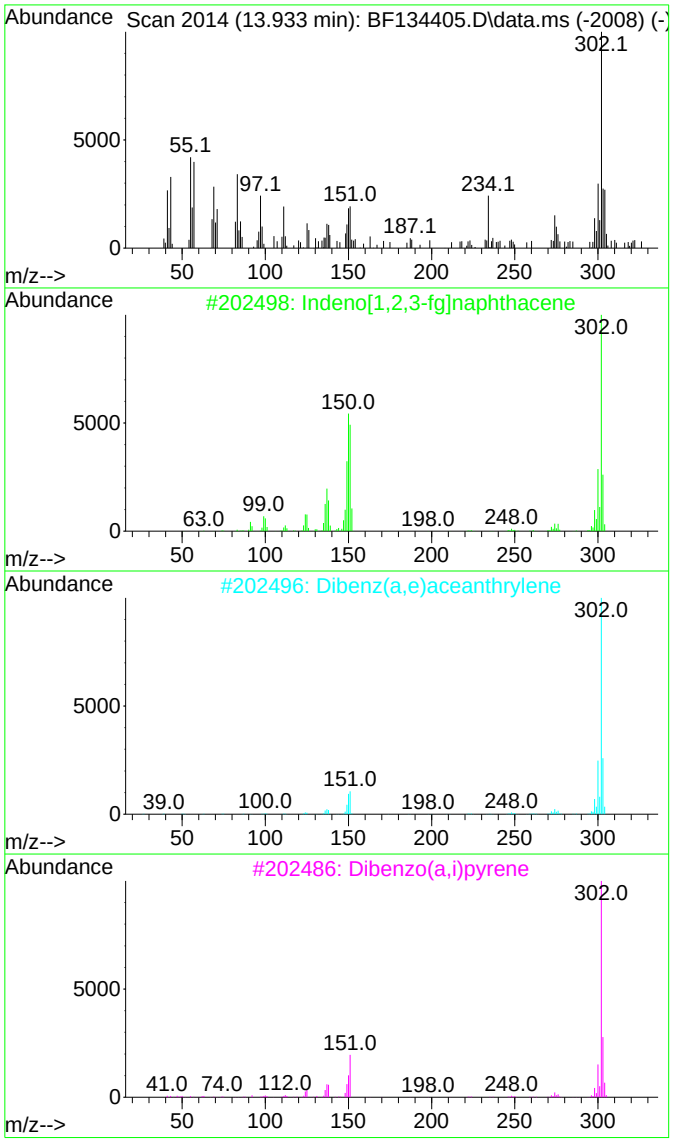
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

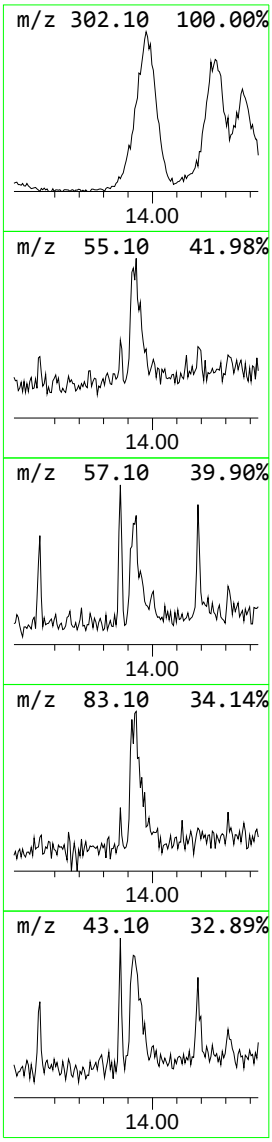
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Indeno[1,2,3-fg]naphthacene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.933	3.63 ng	92049	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indeno[1,2,3-fg]naphthacene	302	C24H14	000203-11-2	78
2	Dibenz(a,e)aceanthrylene	302	C24H14	005385-75-1	53
3	Dibenzo(a,i)pyrene	302	C24H14	000189-55-9	49
4	1,2:4,5-Dibenzopyrene	302	C24H14	000192-65-4	47
5	Benzo[4,5]thiazolo[2,3-c][1,2,4]...	302	C15H6N6S	1000303-95-5	46





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Data File : BF134405.D
Acq On : 21 Jul 2023 17:19
Operator : CG\JU
Sample : 03640-21
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

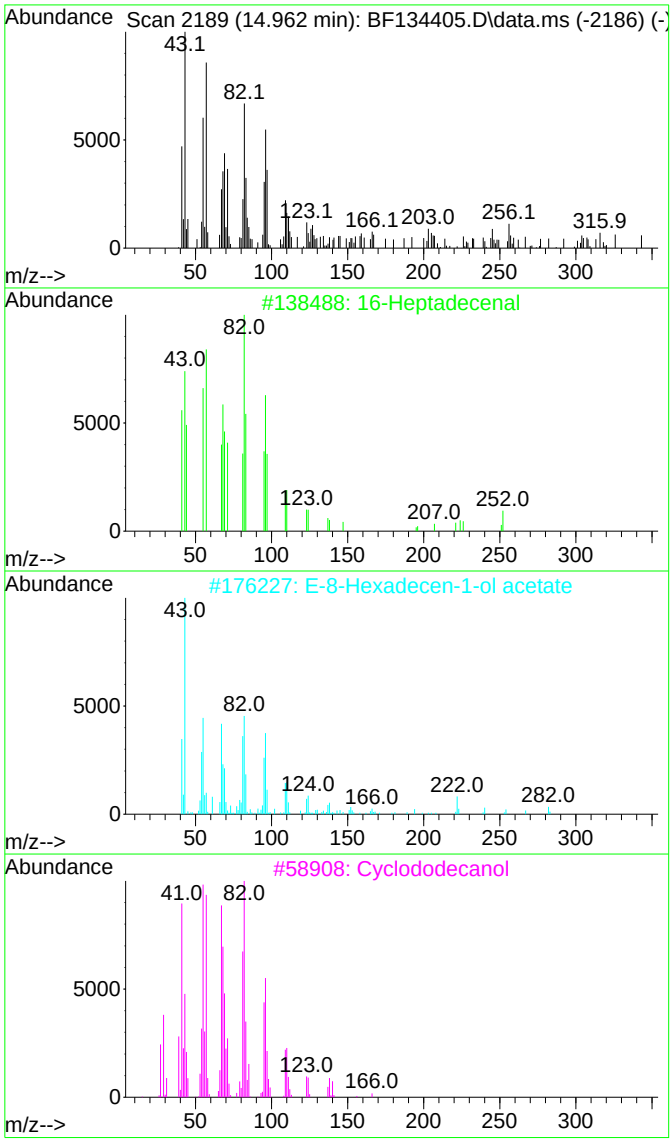
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

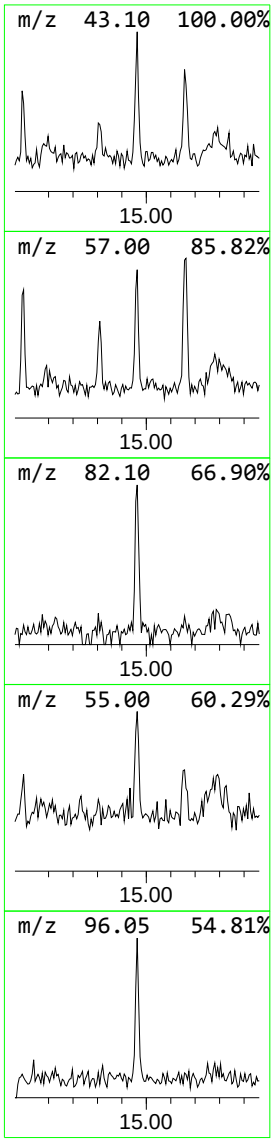
****

Peak Number 7 16-Heptadecenal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.962	2.26 ng	41147	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Heptadecenal	252	C17H32O	1010144-57-9	64
2	E-8-Hexadecen-1-ol acetate	282	C18H34O2	1000131-01-1	62
3	Cyclododecanol	184	C12H24O	001724-39-6	59
4	Z-11-Pentadecenol	226	C15H30O	1000130-77-0	55
5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
Data File : BF134405.D
Acq On : 21 Jul 2023 17:19
Operator : CG\JU
Sample : 03640-21
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

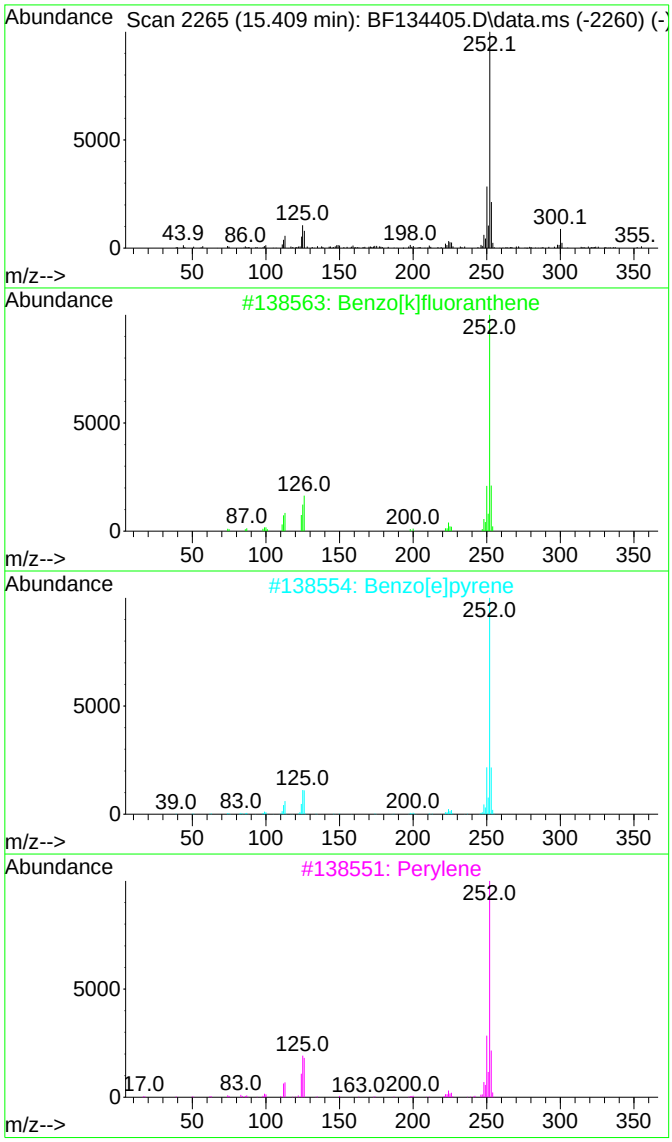
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

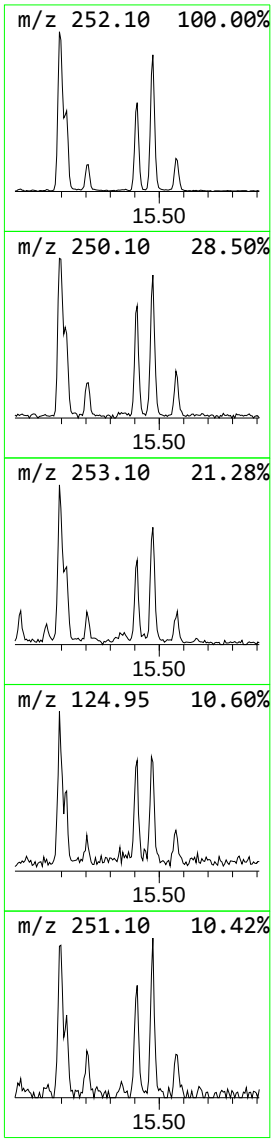
****

Peak Number 8 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.409	7.49 ng	136416	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
2	Benzo[e]pyrene	252	C20H12	000192-97-2	96
3	Perylene	252	C20H12	000198-55-0	95
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Benzo[a]pyrene	252	C20H12	000050-32-8	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
Data File : BF134405.D
Acq On : 21 Jul 2023 17:19
Operator : CG\JU
Sample : 03640-21
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP12

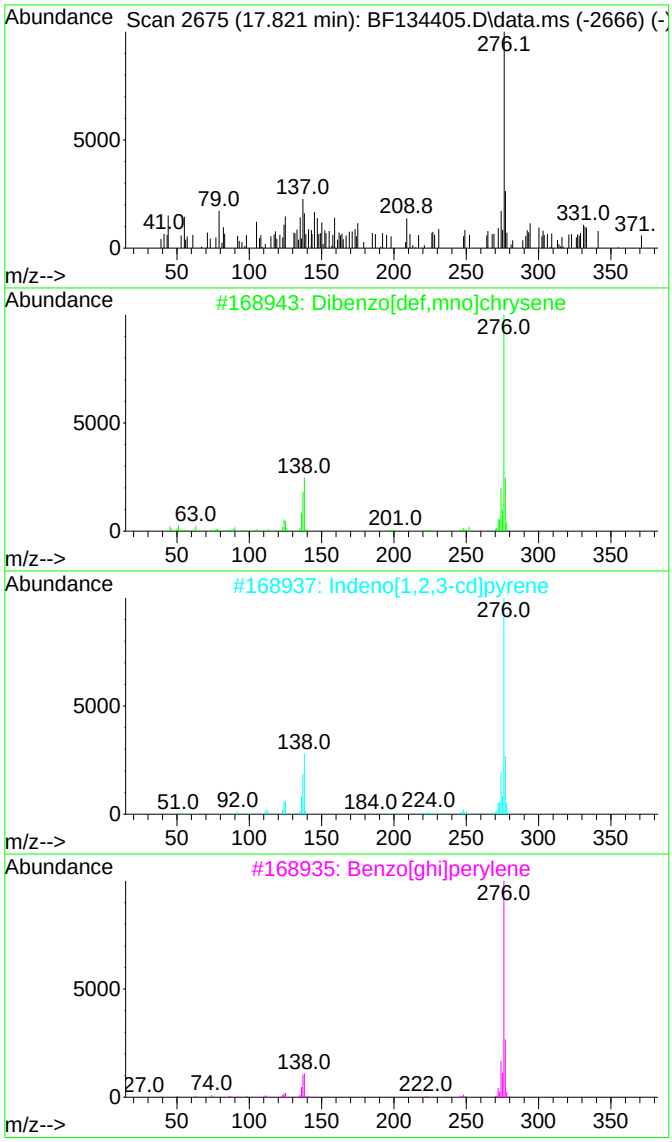
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

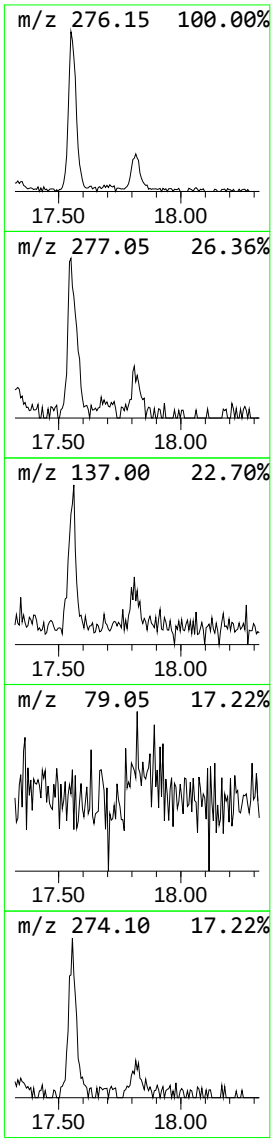
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Dibenzo[def,mno]chrysene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.821	3.09 ng	56223	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	52
2	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	52
3	Benzo[ghi]perylene	276	C22H12	000191-24-2	50
4	Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	47
5	acetonitrile, 2-(3,4-diphenyl-2(...	276	C17H12N2S	1000397-07-9	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
Data File : BF134405.D
Acq On : 21 Jul 2023 17:19
Operator : CG\JU
Sample : 03640-21
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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...	2.151	14.8	ng	264347	1	6.839	358156	20.0
Bicyclo[2.2.1]h...	7.857	2.5	ng	58076	2	8.116	456062	20.0
Anthracene, 9-m...	11.868	2.7	ng	67510	4	11.368	501271	20.0
n-Hexadecanoic ...	11.898	7.8	ng	194415	4	11.368	501271	20.0
4H-Cyclopenta[d...	11.986	2.2	ng	54522	4	11.368	501271	20.0
Indeno[1,2,3-fg...	13.933	3.6	ng	92049	5	14.033	507215	20.0
16-Heptadecenal	14.962	2.3	ng	41147	6	15.539	364237	20.0
Benzo[e]pyrene	15.409	7.5	ng	136416	6	15.539	364237	20.0
Dibenzo[def,mno...	17.821	3.1	ng	56223	6	15.539	364237	20.0