

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
 Data File : BF136893.D
 Acq On : 03 Jan 2024 02:40
 Operator : CG\JU
 Sample : 05899-13
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GHL-SS-13

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136893.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.281	196	203	214	rBV	69616	127935	7.60%	0.753%
2	3.775	281	287	295	rBV	14045	22079	1.31%	0.130%
3	3.869	298	303	308	rVV	101894	129956	7.72%	0.765%
4	5.022	495	499	510	rVB	52846	71998	4.28%	0.424%
5	5.275	538	542	547	rBV	372510	322502	19.16%	1.899%
6	5.381	556	560	562	rBV	829239	881860	52.39%	5.193%
7	5.428	565	568	582	rVB	1560271	1434659	85.23%	8.448%
8	5.634	600	603	607	rBV	131457	122912	7.30%	0.724%
9	5.951	653	657	661	rVB	45473	40871	2.43%	0.241%
10	6.434	734	739	754	rBV	1384794	1480960	87.98%	8.721%
11	6.781	794	798	801	rBV	550444	427684	25.41%	2.519%
12	6.851	808	810	817	rVB	25864	20239	1.20%	0.119%
13	7.345	889	894	897	rBV	937751	923847	54.88%	5.440%
14	8.057	1009	1015	1018	rBV	699640	566656	33.66%	3.337%
15	9.133	1193	1198	1201	rBV	2116070	1683278	100.00%	9.912%
16	9.810	1310	1313	1317	rBV	665517	586338	34.83%	3.453%
17	10.022	1345	1349	1355	rBV3	35567	55431	3.29%	0.326%
18	10.363	1403	1407	1412	rBV2	28975	31847	1.89%	0.188%
19	10.604	1444	1448	1458	rBV	1044947	979068	58.16%	5.765%
20	10.733	1465	1470	1473	rBV2	26185	33229	1.97%	0.196%
21	10.827	1484	1486	1491	rVB	28879	27283	1.62%	0.161%
22	10.974	1508	1511	1520	rBV	61686	75937	4.51%	0.447%
23	11.304	1563	1567	1569	rBV	708774	574876	34.15%	3.385%
24	11.327	1569	1571	1575	rVV	138814	106217	6.31%	0.625%
25	11.380	1575	1580	1583	rVV	155935	131203	7.79%	0.773%
26	11.545	1604	1608	1612	rBV	37520	40552	2.41%	0.239%
27	11.851	1655	1660	1670	rBV	1233038	1495747	88.86%	8.808%
28	12.245	1724	1727	1733	rBV6	29366	45790	2.72%	0.270%
29	12.521	1771	1774	1777	rBV	147767	140204	8.33%	0.826%
30	12.551	1777	1779	1789	rVV4	83302	197698	11.74%	1.164%
31	12.633	1789	1793	1804	rVV	722555	801995	47.64%	4.723%
32	12.751	1808	1813	1816	rVV	111990	128533	7.64%	0.757%
33	12.804	1819	1822	1830	rVB2	35446	53088	3.15%	0.313%
34	12.898	1834	1838	1842	rVV	1435809	1284489	76.31%	7.564%
35	13.633	1960	1963	1971	rBV10	22469	38037	2.26%	0.224%
36	13.733	1977	1980	1983	rBV	303353	294103	17.47%	1.732%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.851	1996	2000	2011	rBV6	53064	134027	7.96%	0.789%
38	13.957	2012	2018	2022	rVV	421743	507225	30.13%	2.987%
39	13.986	2022	2023	2027	rVB	43436	27560	1.64%	0.162%
40	14.433	2096	2099	2103	rBV4	23866	26059	1.55%	0.153%
41	15.004	2193	2196	2200	rBV	66711	96415	5.73%	0.568%
42	15.309	2245	2248	2254	rVB	64204	84435	5.02%	0.497%
43	15.374	2256	2259	2265	rVB	56329	73405	4.36%	0.432%
44	15.439	2265	2270	2274	rBV	314755	401557	23.86%	2.365%
45	15.915	2347	2351	2355	rBV6	18976	27943	1.66%	0.165%
46	16.062	2373	2376	2383	rBV9	15081	32297	1.92%	0.190%
47	16.421	2428	2437	2439	rBV10	13362	37087	2.20%	0.218%
48	16.480	2442	2447	2452	rVB2	16349	33168	1.97%	0.195%
49	16.939	2520	2525	2533	rBV3	25707	55483	3.30%	0.327%
50	17.398	2599	2603	2609	rVB3	17858	34476	2.05%	0.203%
51	17.562	2626	2631	2639	rBV3	12616	31311	1.86%	0.184%

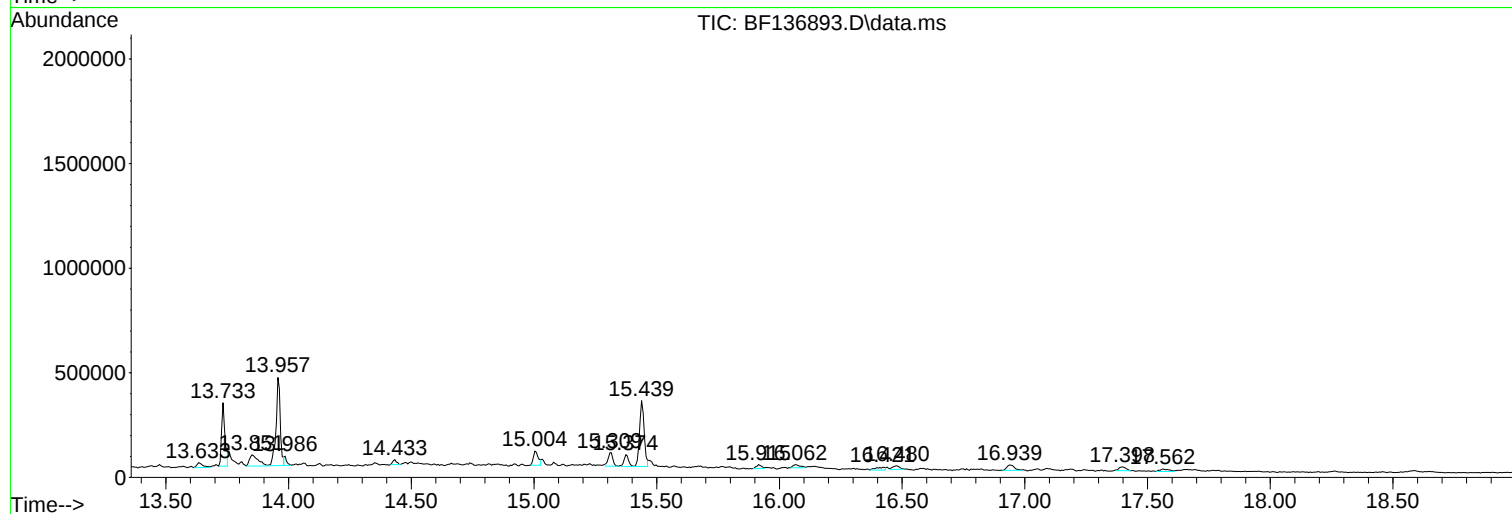
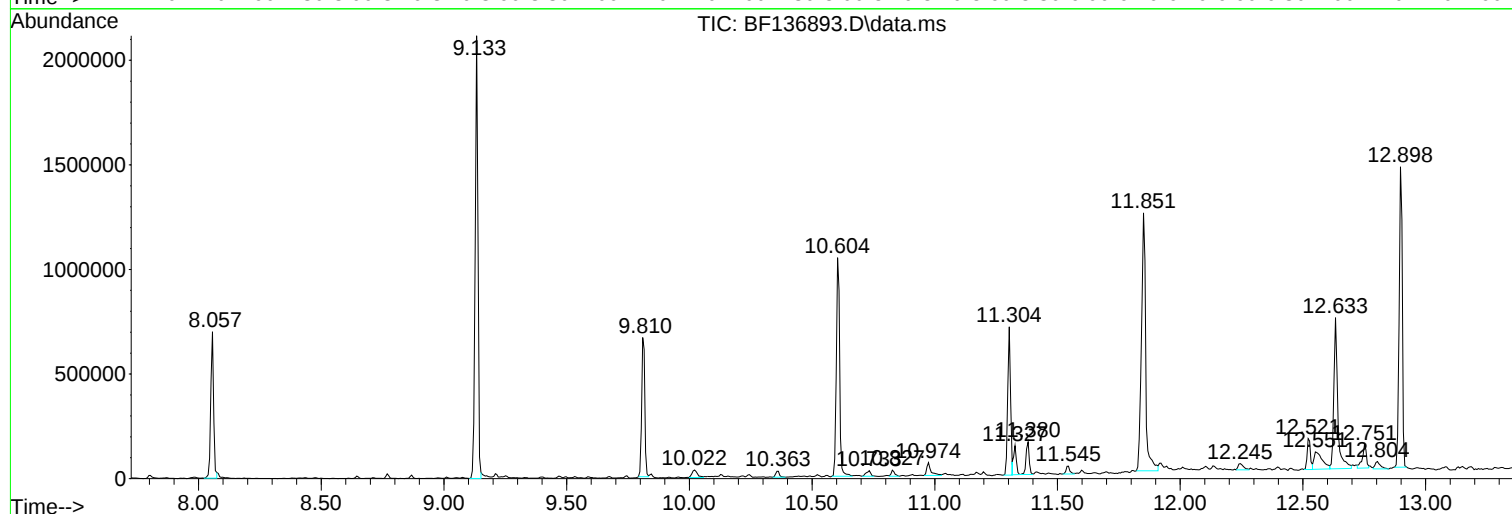
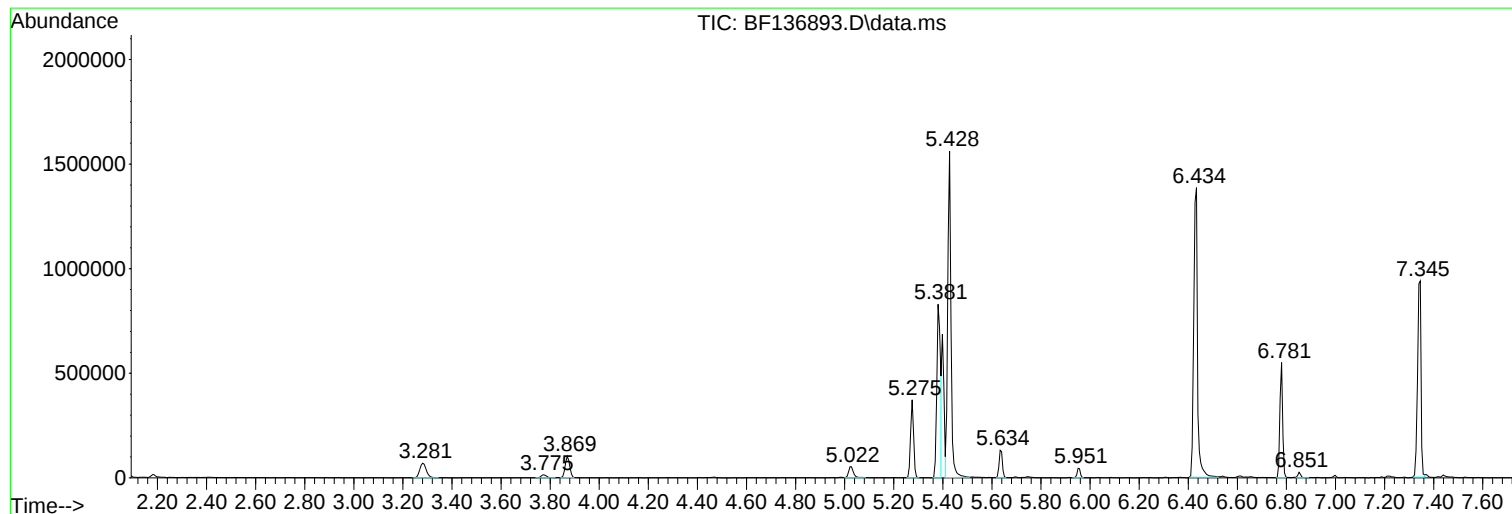
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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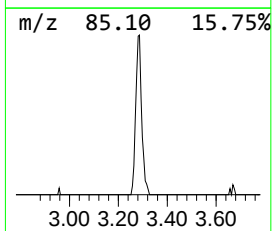
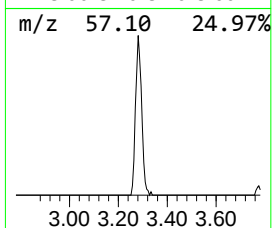
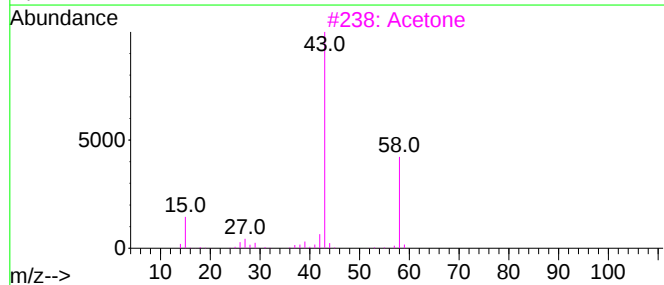
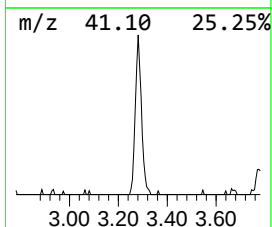
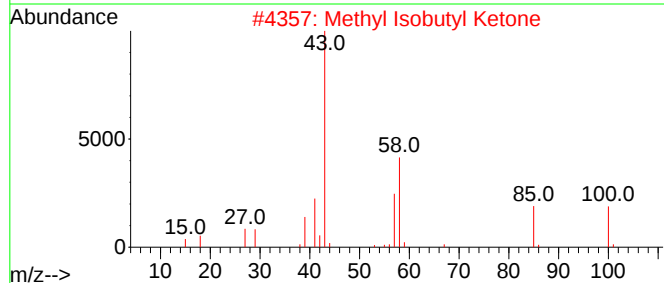
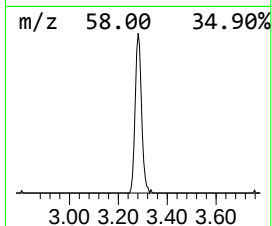
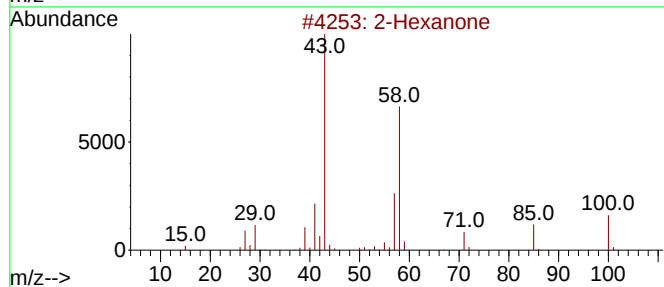
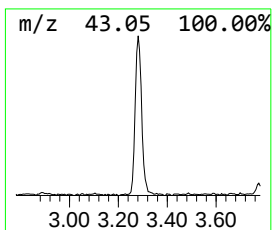
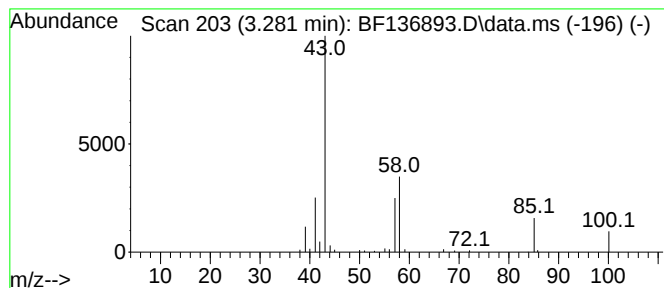
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Hexanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.281	5.98 ng	127935	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hexanone	100	C6H12O	000591-78-6	78
2			Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	78
3			Acetone	58	C3H6O	000067-64-1	38
4			Acetylacetone	100	C5H8O2	000123-54-6	32
5			Oxirane, 2-methyl-2-(1-methyleth...	100	C6H12O	072221-03-5	28



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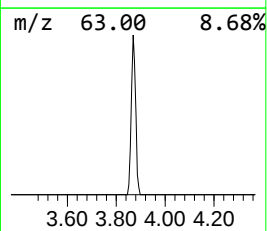
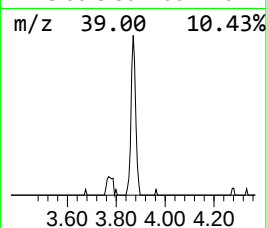
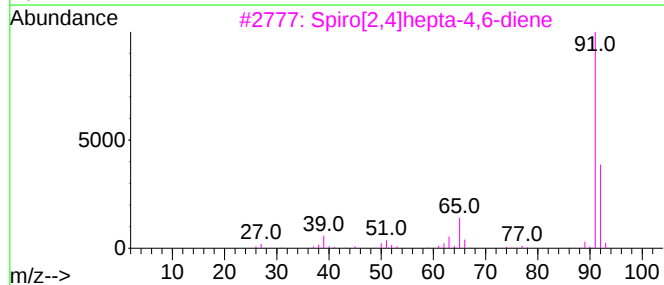
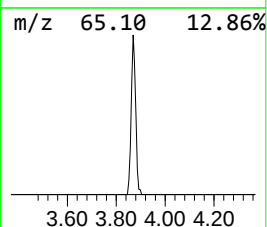
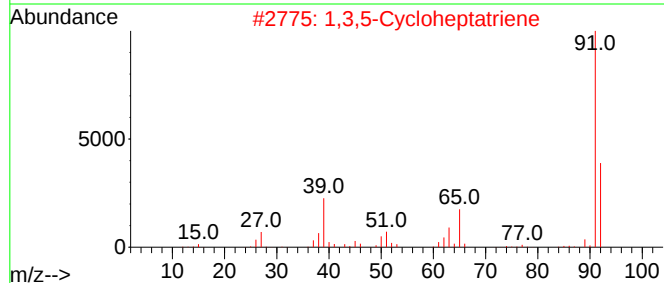
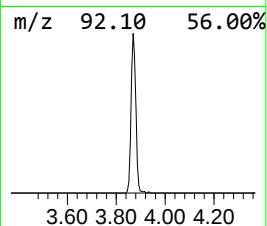
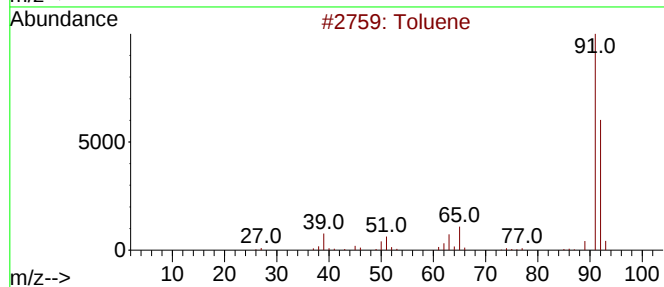
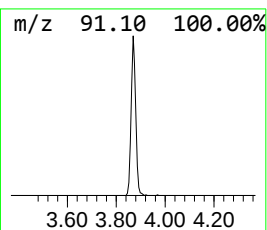
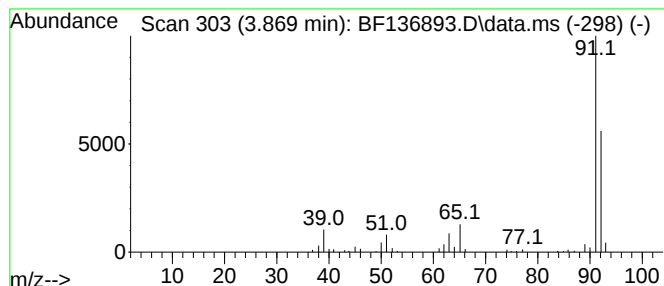
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Toluene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.869	6.08 ng	129956	1,4-Dichlorobenzene-d4	6.781

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Toluene	92	C7H8	000108-88-3	95
2		1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	87
3		Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	87
4		2,5-Norbornadiene	92	C7H8	000121-46-0	83
5		Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	64



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ALS Vial : 19 Sample Multiplier: 1

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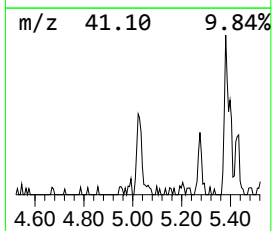
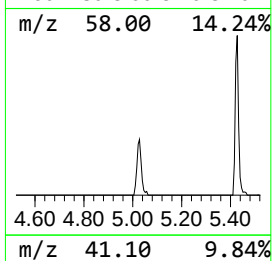
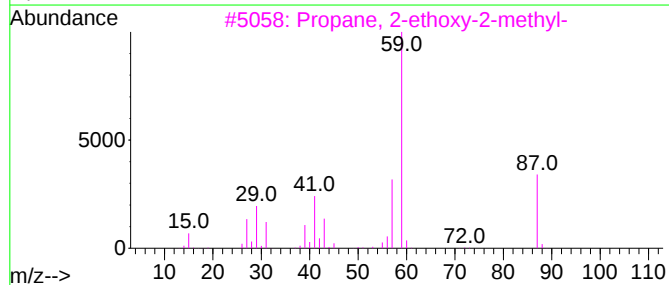
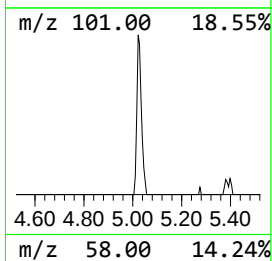
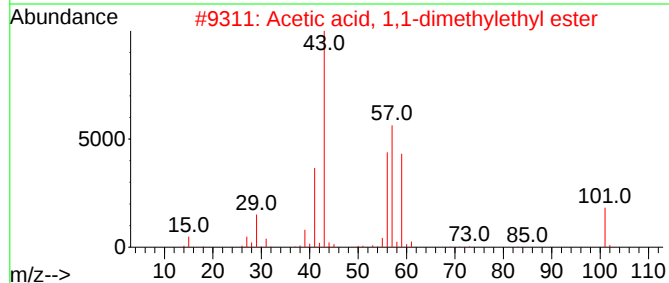
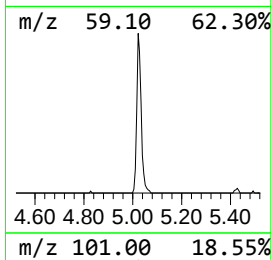
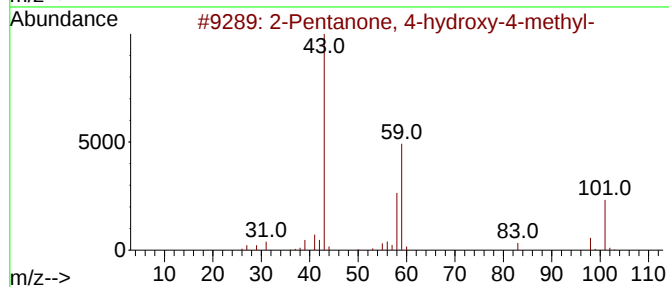
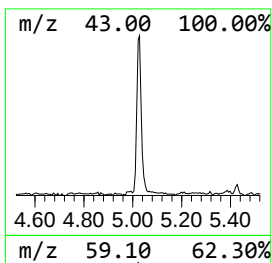
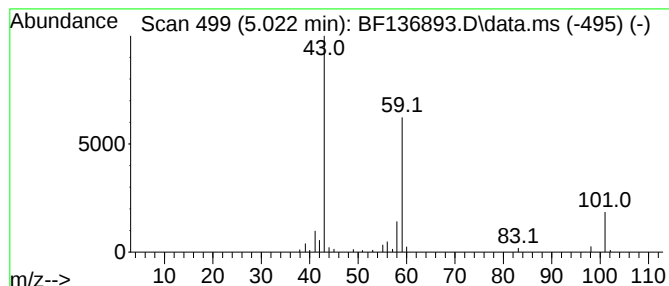
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	3.37 ng	71998	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	25
4			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



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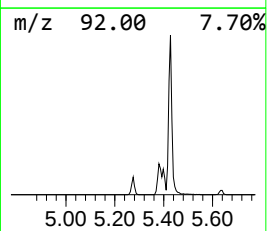
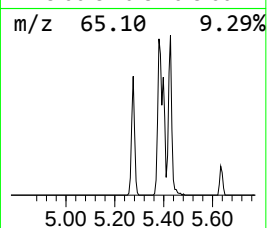
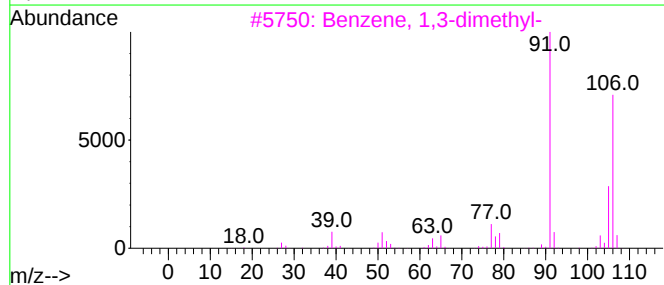
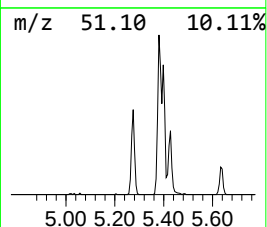
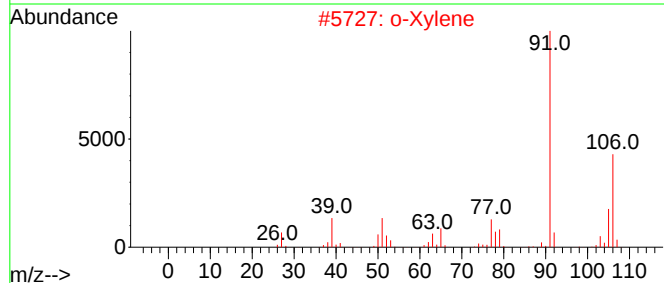
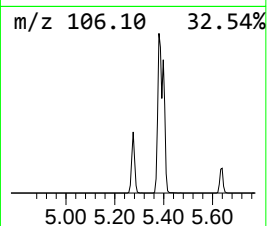
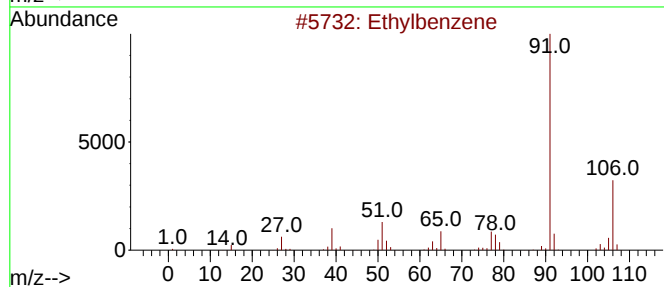
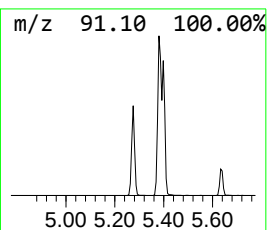
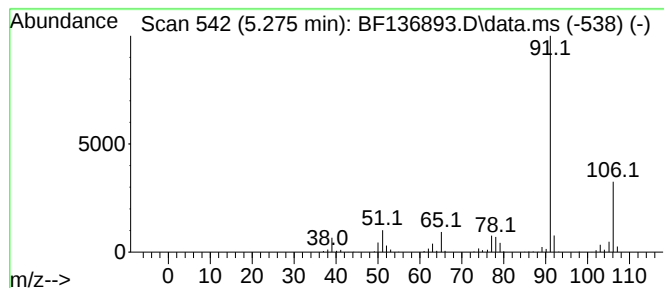
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Ethylbenzene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.275	15.08 ng	322502	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethylbenzene	106	C8H10	000100-41-4	94
2			o-Xylene	106	C8H10	000095-47-6	76
3			Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	72
4			p-Xylene	106	C8H10	000106-42-3	68
5			1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	52



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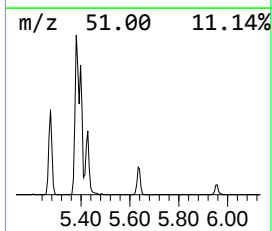
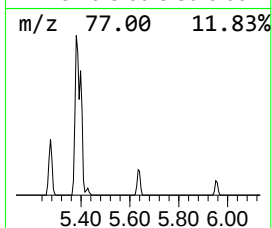
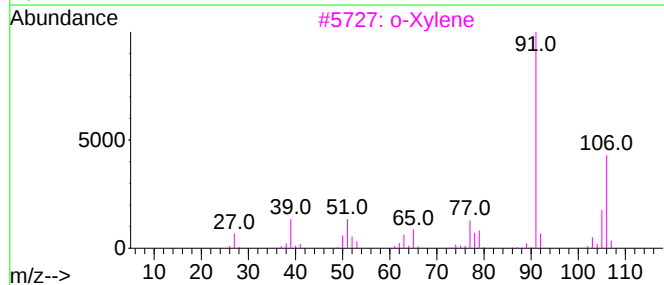
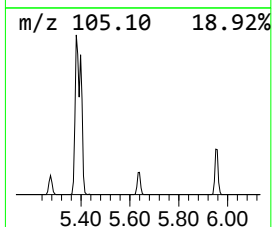
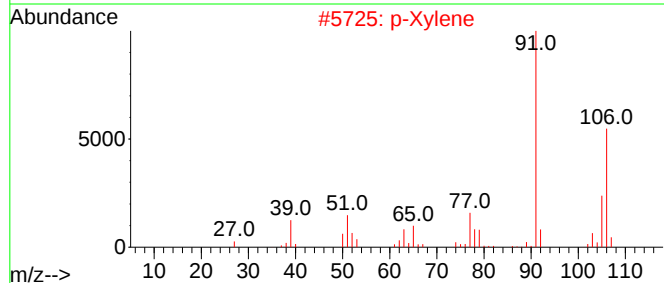
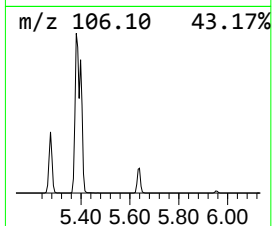
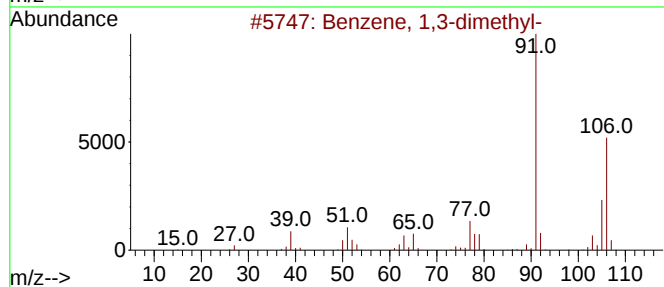
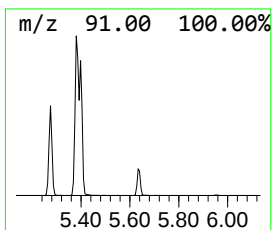
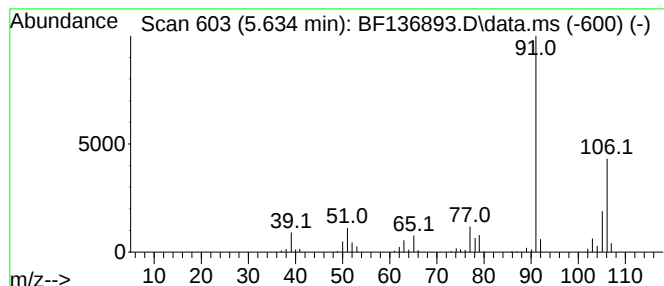
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzene, 1,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.634	5.75 ng	122912	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	97
2			p-Xylene	106	C8H10	000106-42-3	97
3			o-Xylene	106	C8H10	000095-47-6	97
4			1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	91
5			Ethylbenzene	106	C8H10	000100-41-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
Data File : BF136893.D
Acq On : 03 Jan 2024 02:40
Operator : CG\JU
Sample : 05899-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-13

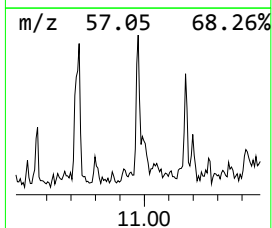
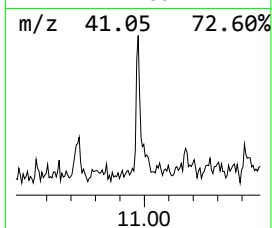
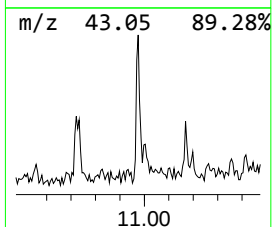
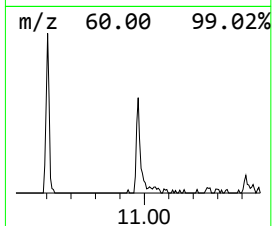
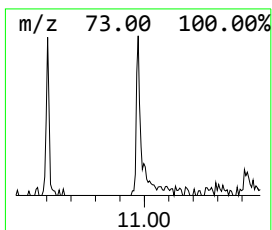
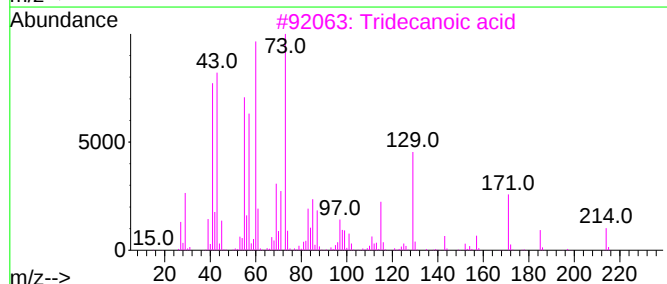
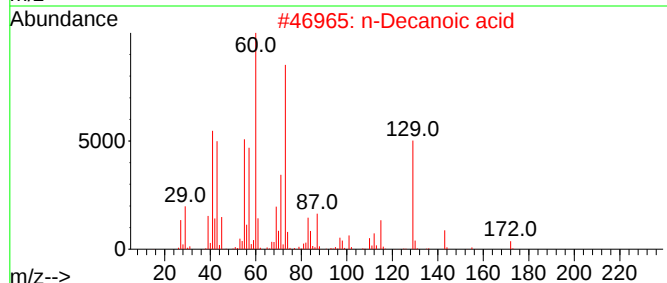
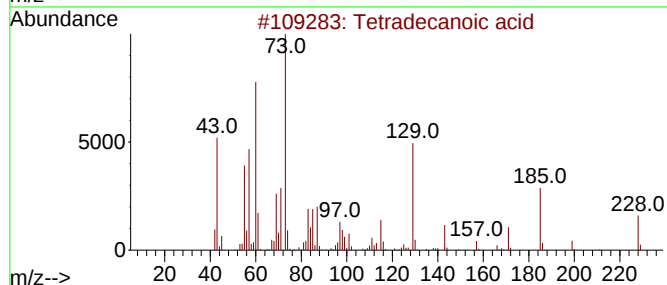
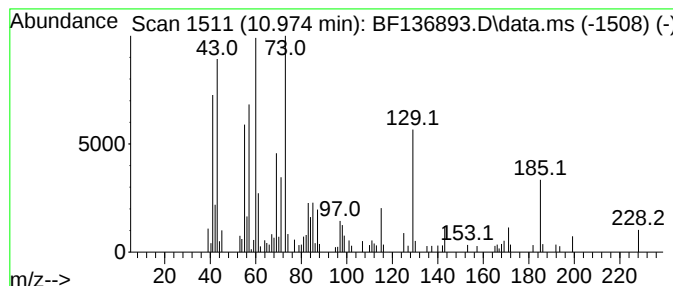
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetradecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.974	2.64 ng	75937	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
2			n-Decanoic acid	172	C10H20O2	000334-48-5	70
3			Tridecanoic acid	214	C13H26O2	000638-53-9	58
4			Dodecanoic acid	200	C12H24O2	000143-07-7	58
5			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NO5	029926-41-8	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
Data File : BF136893.D
Acq On : 03 Jan 2024 02:40
Operator : CG\JU
Sample : 05899-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

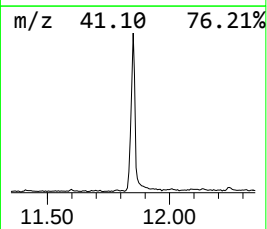
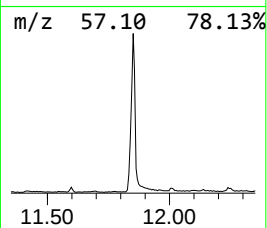
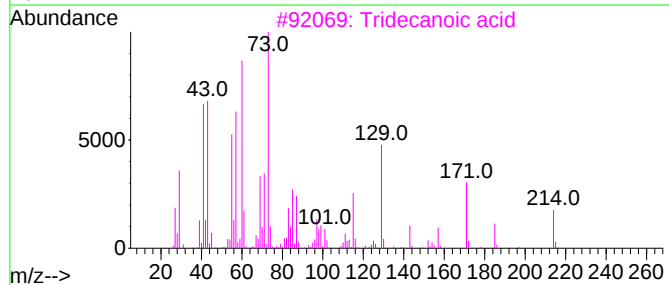
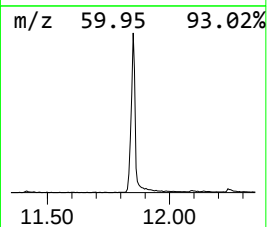
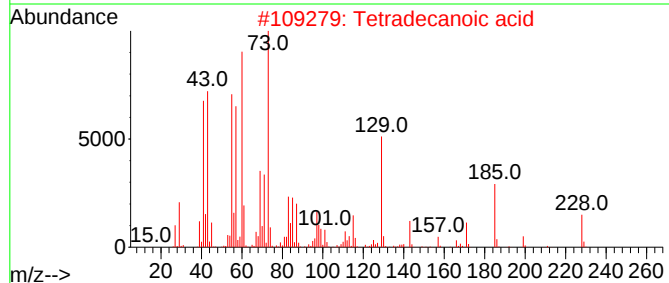
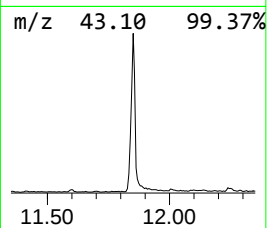
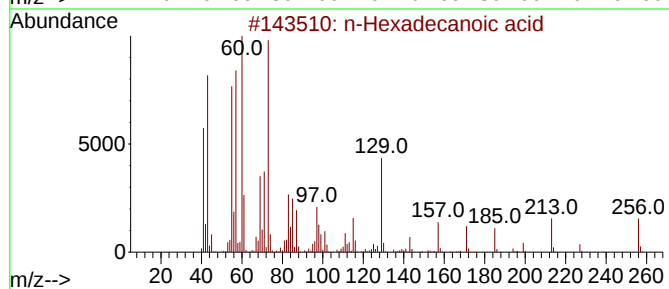
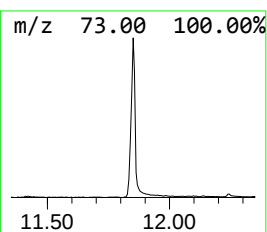
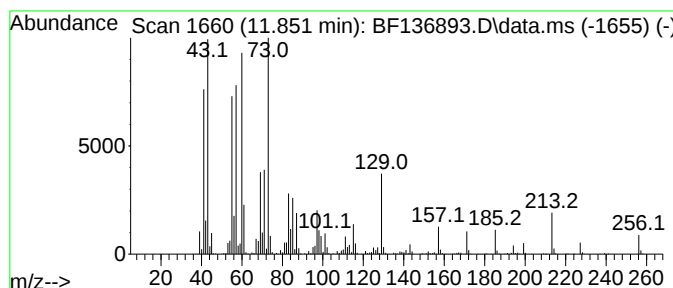
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.851	52.04 ng	1495750	Phenanthrene-d10	11.304	
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	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5	Nonanoic acid	158	C9H18O2	000112-05-0	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
Data File : BF136893.D
Acq On : 03 Jan 2024 02:40
Operator : CG\JU
Sample : 05899-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-13

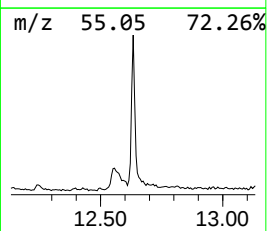
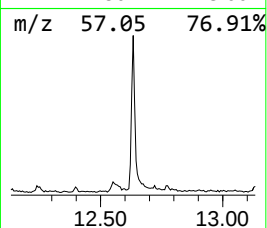
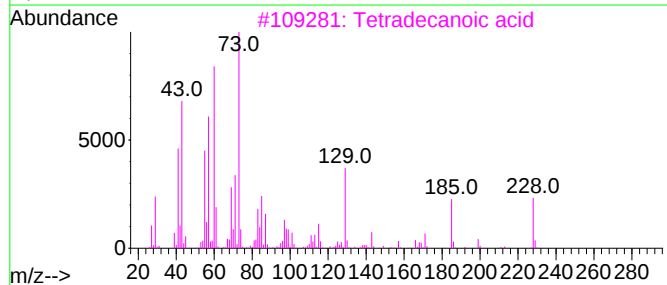
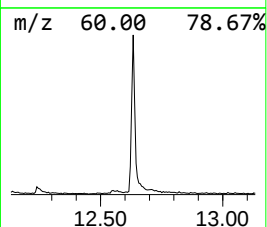
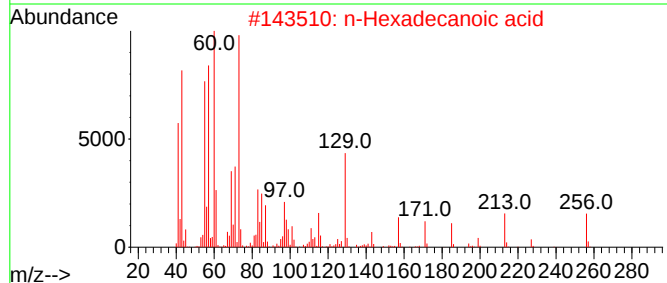
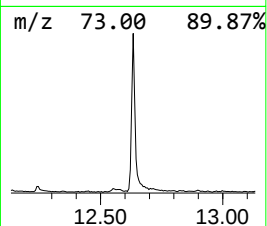
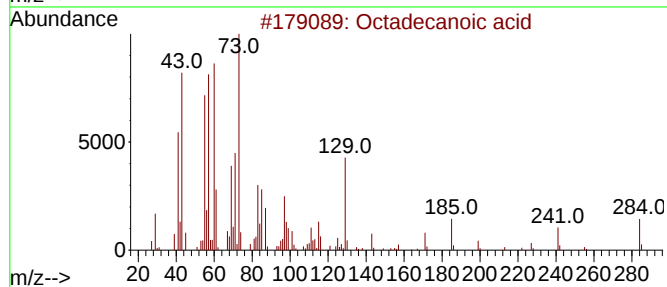
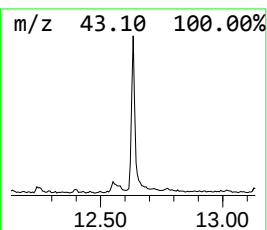
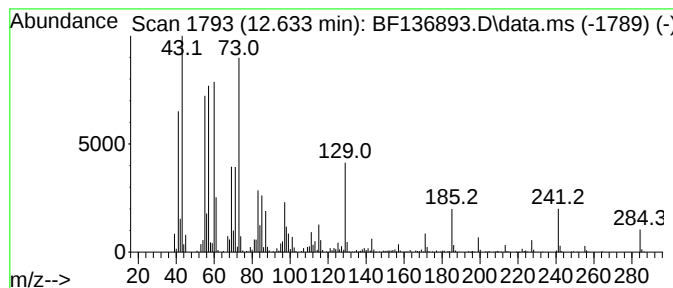
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.633	31.62 ng	801995	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5			Tridecanoic acid	214	C13H26O2	000638-53-9	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
Data File : BF136893.D
Acq On : 03 Jan 2024 02:40
Operator : CG\JU
Sample : 05899-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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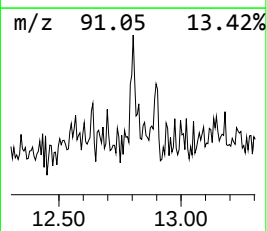
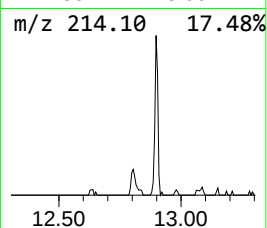
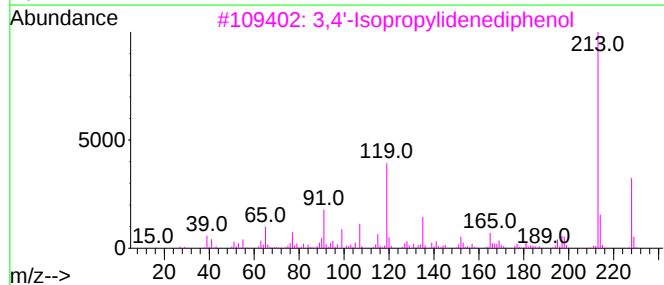
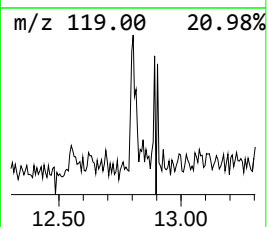
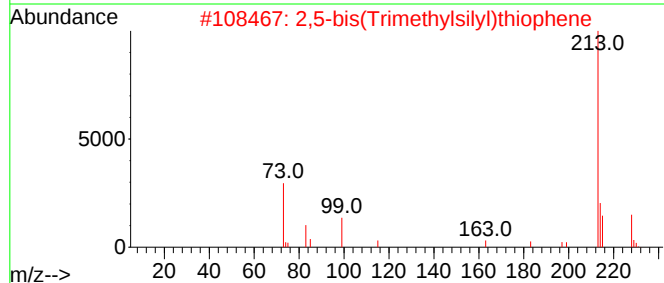
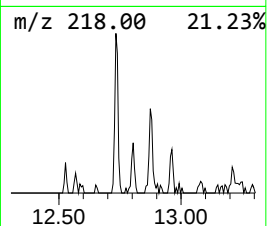
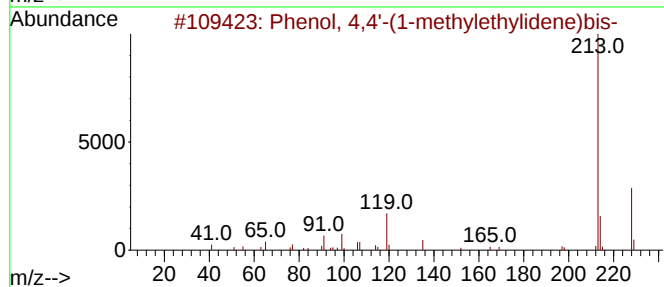
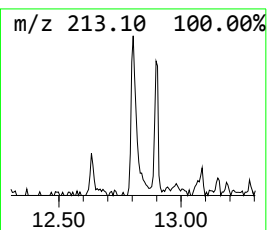
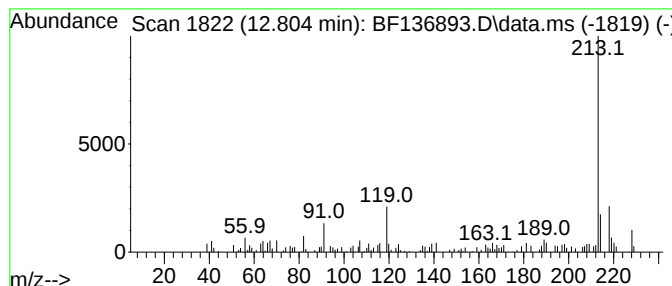
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Phenol, 4,4'-(1-methylethyl... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.804	2.09 ng	53088	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	64
2			2,5-bis(Trimethylsilyl)thiophene	228	C10H20SSi2	017906-71-7	53
3			3,4'-Isopropylidenediphenol	228	C15H16O2	046765-25-7	53
4			2,4(1H,3H)-Pyrimidinedione, 1,3-...	228	C9H16N2O3Si	089447-84-7	50
5			2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
Data File : BF136893.D
Acq On : 03 Jan 2024 02:40
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ClientSampleId :
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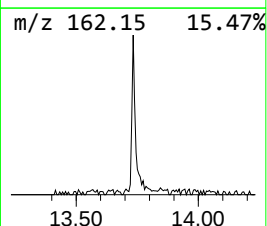
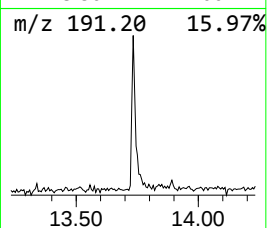
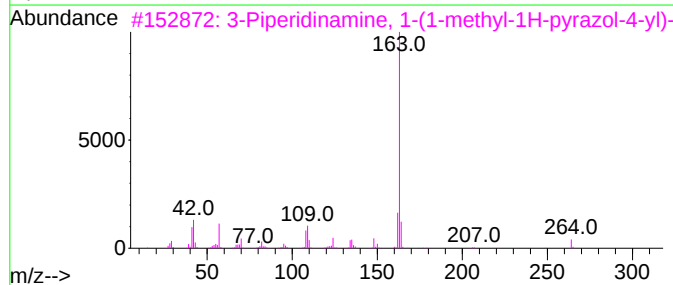
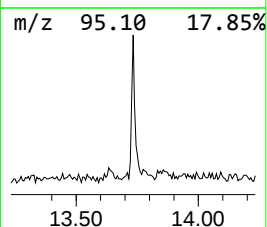
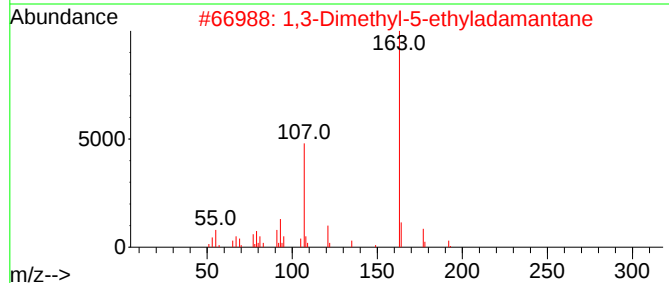
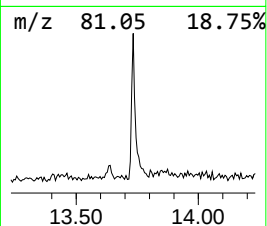
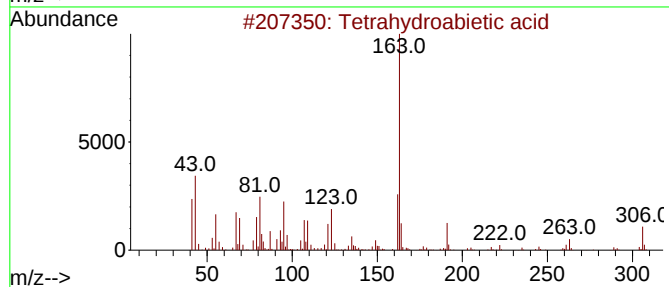
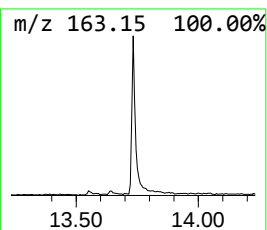
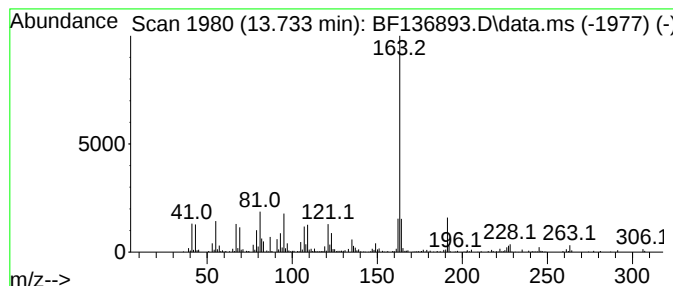
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetrahydroabietic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.733	11.60 ng	294103	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetrahydroabietic acid	306	C20H34O2	1000251-96-9	64
2			1,3-Dimethyl-5-ethyladamantane	192	C14H24	001687-35-0	53
3			3-Piperidinamine, 1-(1-methyl-1H...	264	C14H24N4O	1000470-29-4	53
4			Benzamide, 2-hydroxy-N-[4-hydro...	299	C18H21NO3	1000350-33-6	53
5			3-Piperidinamine, 1-(1-methyl-1H...	250	C13H22N4O	1010470-28-9	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
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Operator : CG\JU
Sample : 05899-13
Misc :
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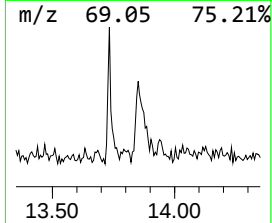
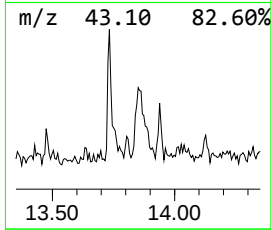
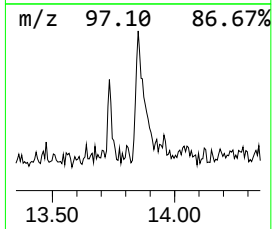
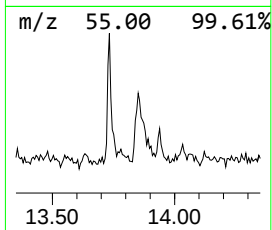
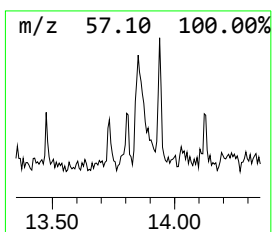
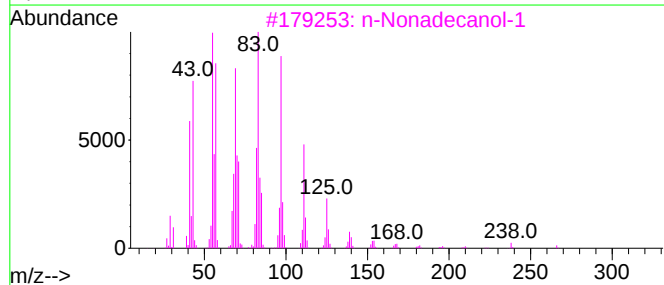
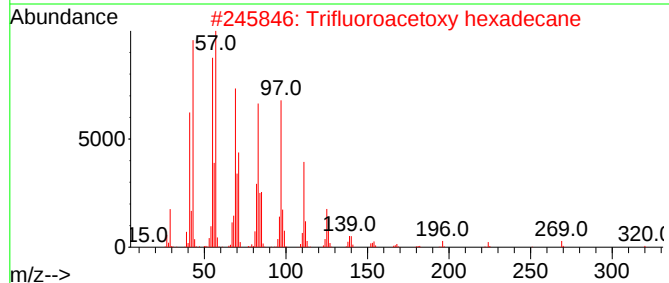
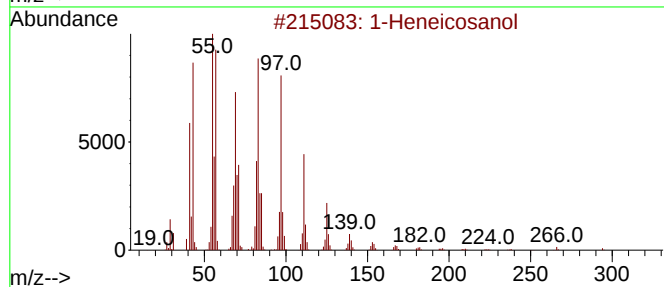
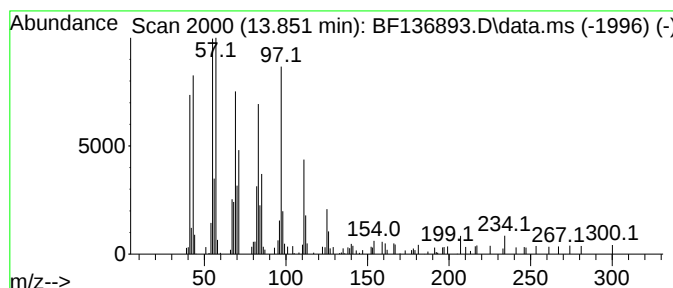
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Heneicosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.851	5.28 ng	134027	Chrysene-d12	13.957	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	90
4	Behenic alcohol	326	C22H46O	000661-19-8	90
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
Data File : BF136893.D
Acq On : 03 Jan 2024 02:40
Operator : CG\JU
Sample : 05899-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-13

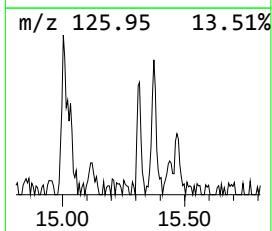
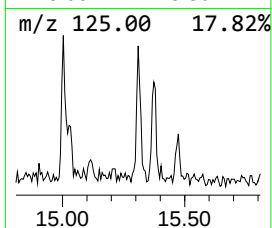
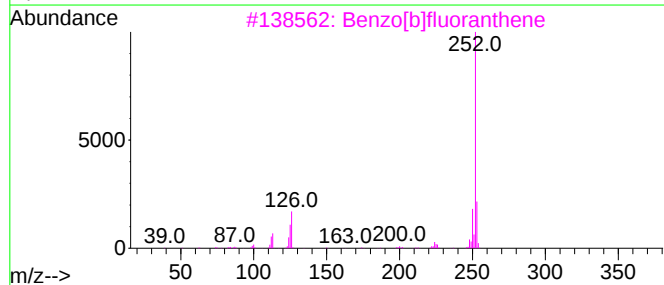
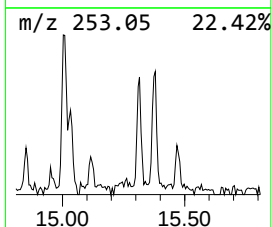
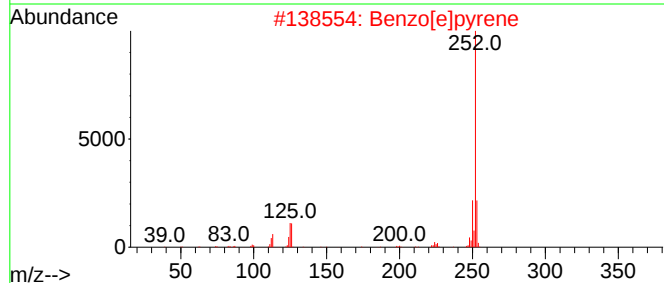
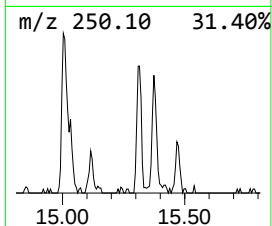
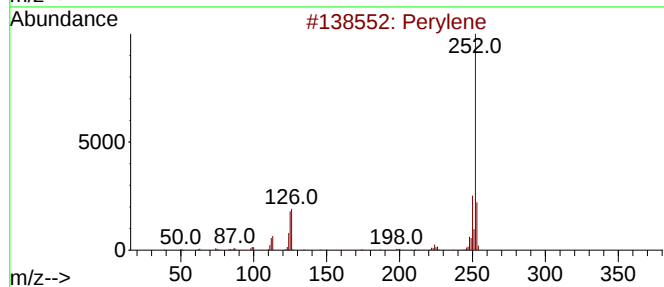
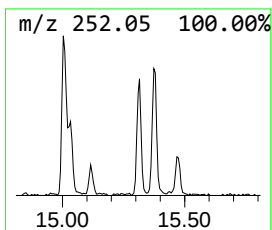
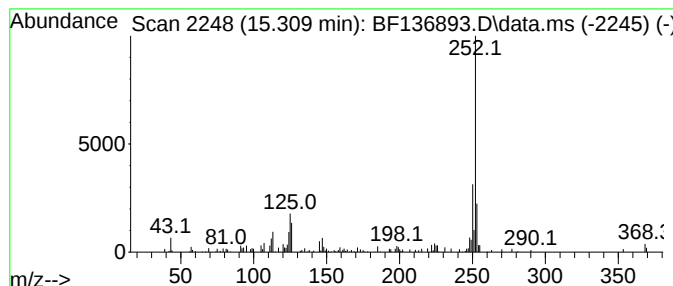
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Perylene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.309	4.21 ng	84435	Perylene-d12	15.439

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Perylene	252	C20H12	000198-55-0	96
2		Benzo[e]pyrene	252	C20H12	000192-97-2	96
3		Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
4		Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
5		Benzo[a]pyrene	252	C20H12	000050-32-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
Data File : BF136893.D
Acq On : 03 Jan 2024 02:40
Operator : CG\JU
Sample : 05899-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Hexanone	3.281	6.0	ng	127935	1	6.781	427684	20.0
Toluene	3.869	6.1	ng	129956	1	6.781	427684	20.0
2-Pentanone, 4-...	5.022	3.4	ng	71998	1	6.781	427684	20.0
Ethylbenzene	5.275	15.1	ng	322502	1	6.781	427684	20.0
Benzene, 1,3-di...	5.634	5.8	ng	122912	1	6.781	427684	20.0
Tetradecanoic acid	10.974	2.6	ng	75937	4	11.304	574876	20.0
n-Hexadecanoic ...	11.851	52.0	ng	1495750	4	11.304	574876	20.0
Octadecanoic acid	12.633	31.6	ng	801995	5	13.957	507225	20.0
Phenol, 4,4'-(1...	12.804	2.1	ng	53088	5	13.957	507225	20.0
Tetrahydroabiet...	13.733	11.6	ng	294103	5	13.957	507225	20.0
1-Heneicosanol	13.851	5.3	ng	134027	5	13.957	507225	20.0
Perylene	15.309	4.2	ng	84435	6	15.439	401557	20.0