

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072523\
 Data File : BF134474.D
 Acq On : 25 Jul 2023 21:23
 Operator : CG\JU
 Sample : 03654-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-12016

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-BF072423.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134474.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	3	15	21	rVB	199538	294019	8.84%	1.266%
2	5.104	510	513	525	rVB	34913	50552	1.52%	0.218%
3	5.481	573	577	599	rBV	3008095	2935867	88.25%	12.645%
4	6.481	742	747	750	rBV	2965431	2890315	86.88%	12.448%
5	6.834	803	807	817	rBV	748920	666482	20.03%	2.870%
6	7.398	899	903	906	rBV	2036013	1814148	54.53%	7.813%
7	8.110	1021	1024	1036	rBV	1119234	845783	25.42%	3.643%
8	9.186	1203	1207	1211	rBV	3508695	3326781	100.00%	14.328%
9	9.492	1256	1259	1262	rBV	83393	65547	1.97%	0.282%
10	9.586	1270	1275	1279	rVB2	71803	82397	2.48%	0.355%
11	9.869	1319	1323	1326	rBV	985222	771028	23.18%	3.321%
12	9.898	1326	1328	1337	rVB	38244	34145	1.03%	0.147%
13	10.663	1454	1458	1472	rBV	1906776	1713217	51.50%	7.379%
14	11.363	1573	1577	1579	rBV	732354	585059	17.59%	2.520%
15	11.386	1579	1581	1585	rVV	427131	324736	9.76%	1.399%
16	11.439	1587	1590	1593	rVB	74493	65724	1.98%	0.283%
17	11.869	1659	1663	1665	rBV	39439	36890	1.11%	0.159%
18	11.892	1665	1667	1674	rVB3	128687	143404	4.31%	0.618%
19	11.980	1679	1682	1684	rBV	84390	75936	2.28%	0.327%
20	12.198	1716	1719	1724	rVB	41497	38479	1.16%	0.166%
21	12.457	1760	1763	1769	rVB3	25250	36133	1.09%	0.156%
22	12.586	1781	1785	1789	rBV	551728	530567	15.95%	2.285%
23	12.816	1818	1824	1830	rVB	605314	600072	18.04%	2.584%
24	12.963	1842	1849	1852	rBV	2592922	2458871	73.91%	10.590%
25	13.145	1873	1880	1884	rBV	70763	98675	2.97%	0.425%
26	13.216	1889	1892	1894	rVB	48874	43086	1.30%	0.186%
27	13.251	1894	1898	1900	rBV3	39218	38442	1.16%	0.166%
28	13.774	1984	1987	1989	rBV	56428	54651	1.64%	0.235%
29	13.880	1999	2005	2012	rVB6	77664	148702	4.47%	0.640%
30	14.027	2021	2030	2032	rBV2	645685	840595	25.27%	3.620%
31	14.051	2032	2034	2042	rVV	257889	248763	7.48%	1.071%
32	14.127	2042	2047	2050	rVB2	49292	60294	1.81%	0.260%
33	14.415	2094	2096	2101	rBV2	32103	52193	1.57%	0.225%
34	14.592	2124	2126	2128	rBV3	30532	34661	1.04%	0.149%
35	14.668	2135	2139	2140	rBV3	39964	43743	1.31%	0.188%
36	14.698	2142	2144	2150	rVB3	60292	93394	2.81%	0.402%

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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

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
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37	15.086	2206	2210	2213	rBV	145649	205117	6.17%	0.883%
38	15.398	2259	2263	2269	rVB	82281	106003	3.19%	0.457%
39	15.468	2270	2275	2281	rBV	104337	164975	4.96%	0.711%
40	15.527	2281	2285	2289	rBV	293802	393376	11.82%	1.694%
41	15.992	2361	2364	2367	rBV4	24718	37585	1.13%	0.162%
42	17.068	2544	2547	2553	rBV2	45811	78896	2.37%	0.340%
43	17.545	2624	2628	2637	rVB2	35937	89095	2.68%	0.384%

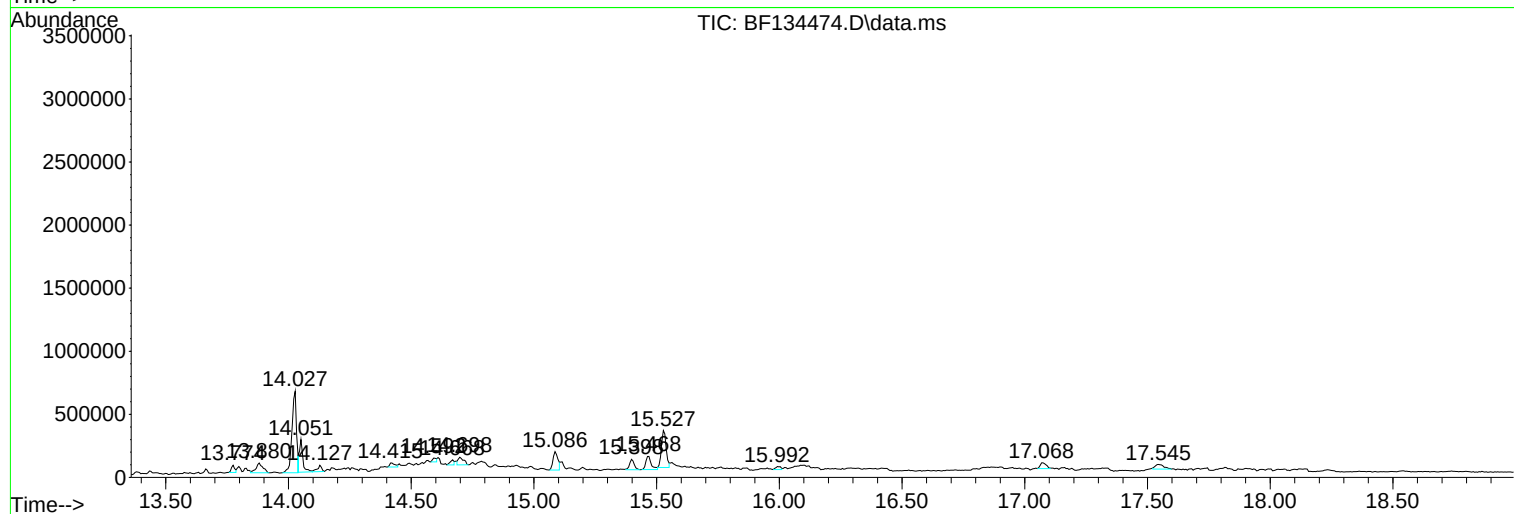
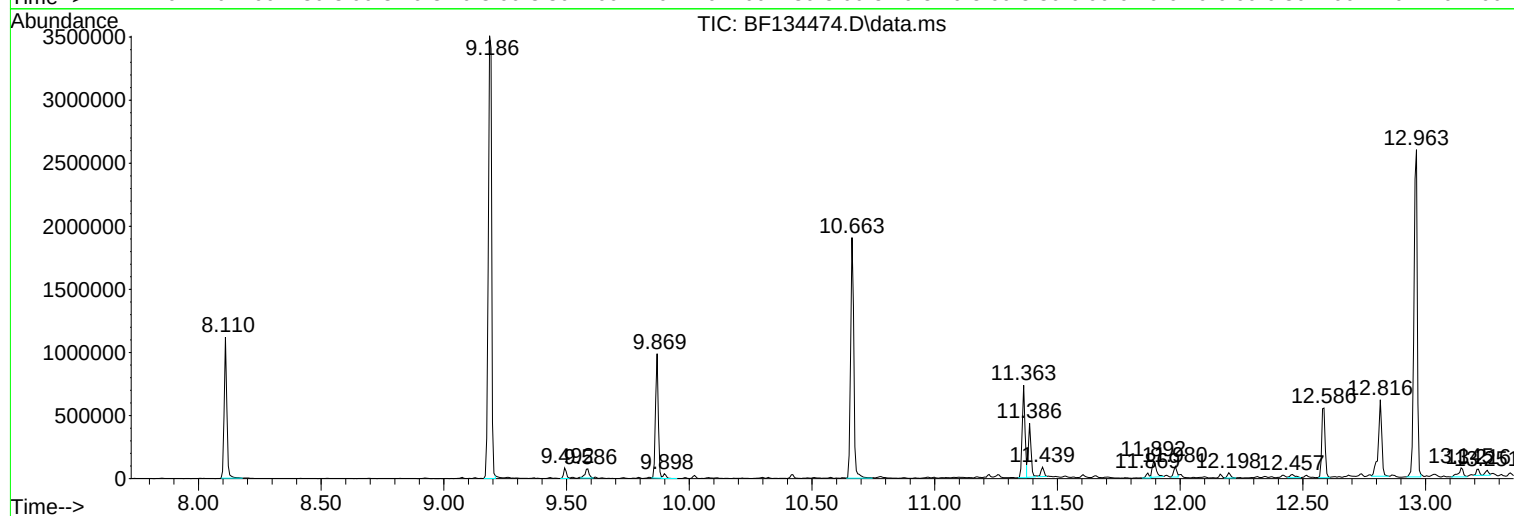
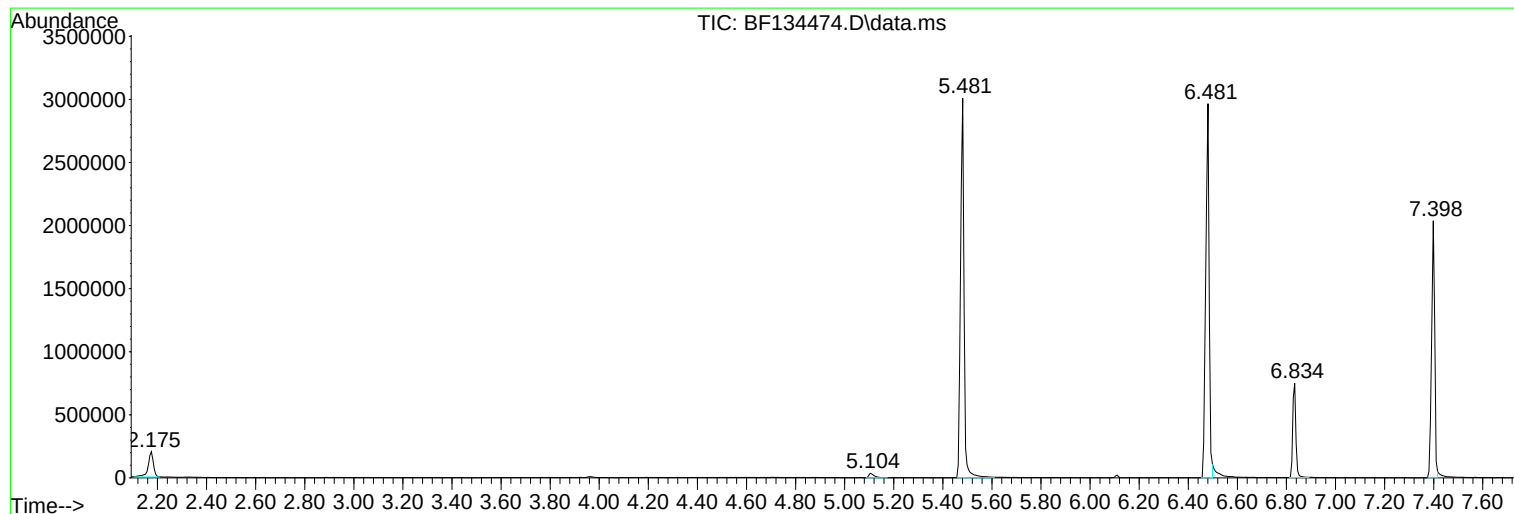
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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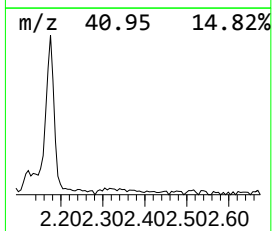
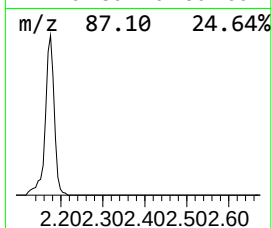
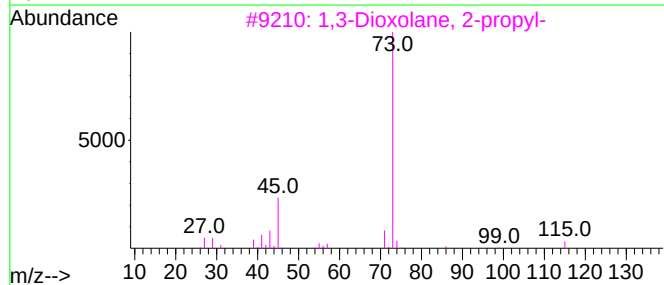
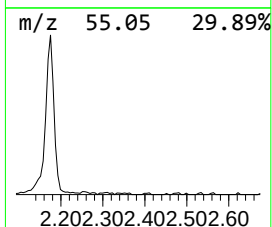
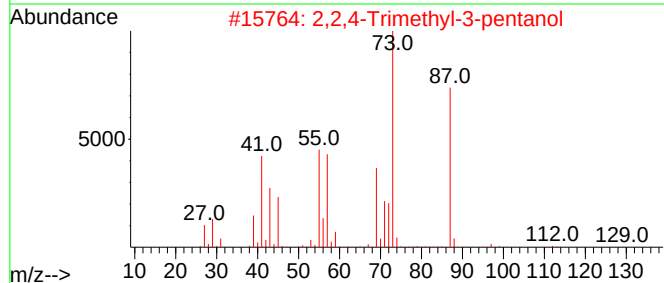
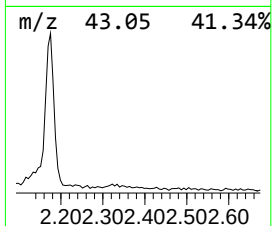
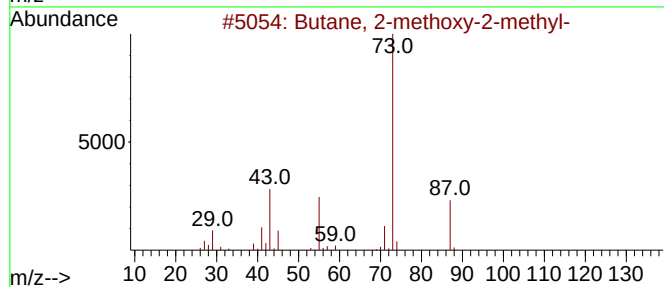
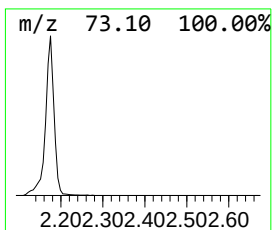
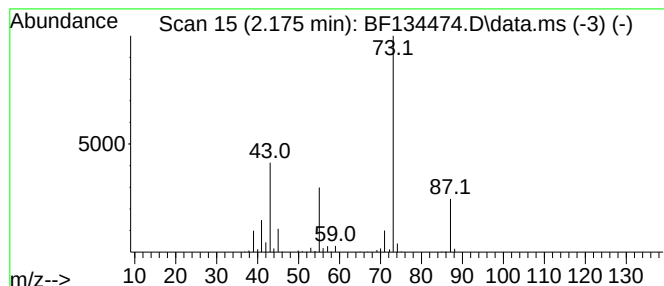
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.175	8.82 ng	294019	1,4-Dichlorobenzene-d4	6.834

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			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23
5			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	23



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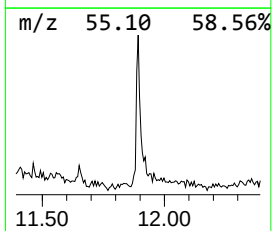
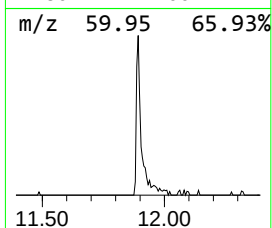
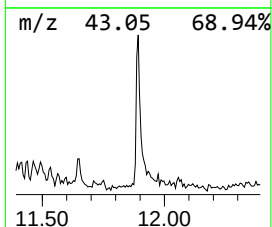
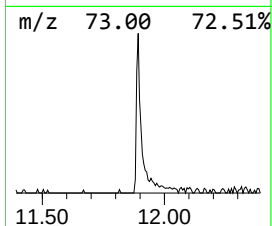
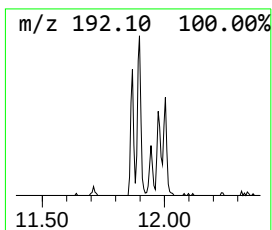
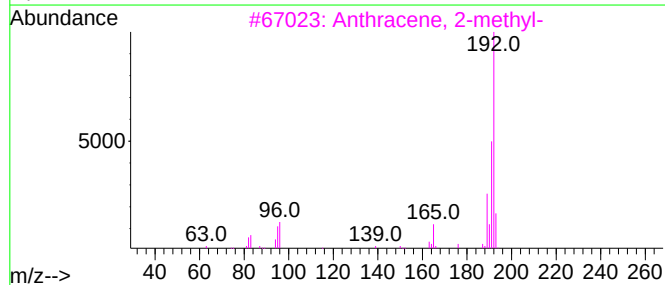
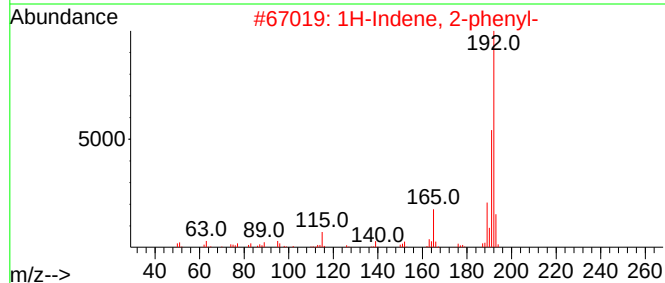
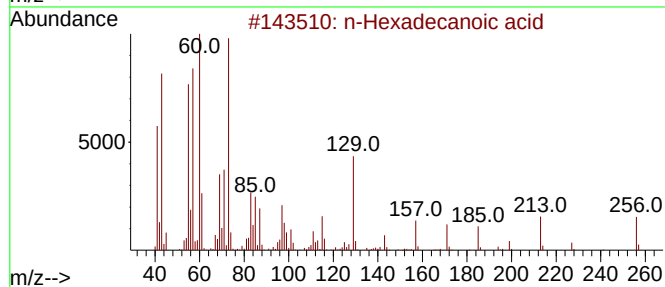
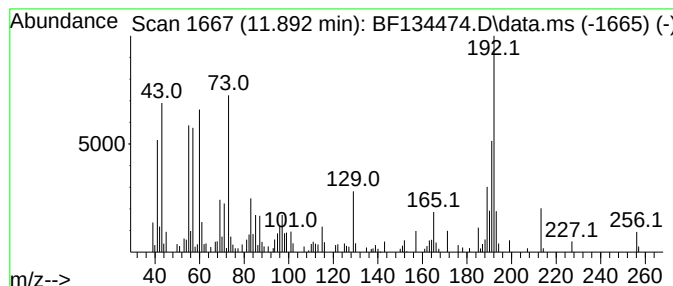
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	4.90 ng	143404	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2			1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	86
3			Anthracene, 2-methyl-	192	C15H12	000613-12-7	78
4			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	70
5			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	70



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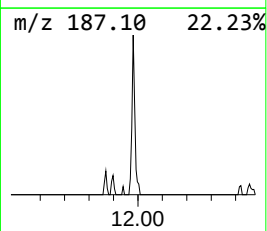
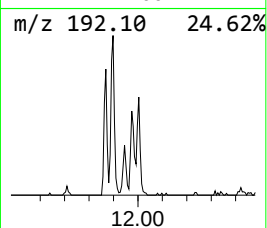
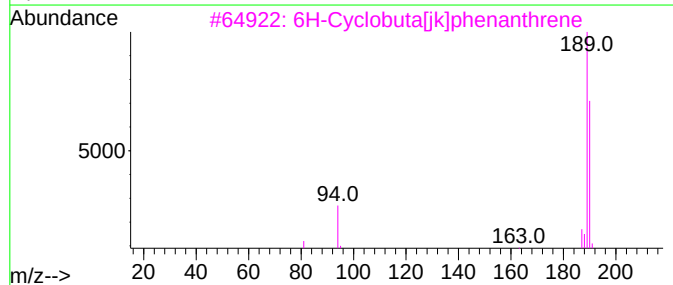
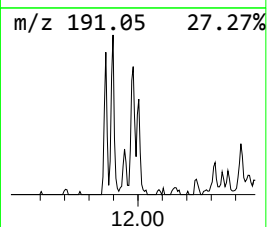
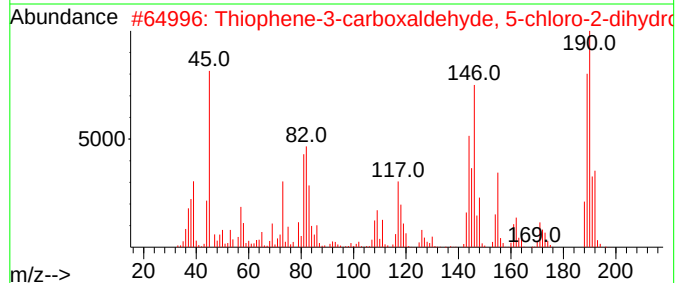
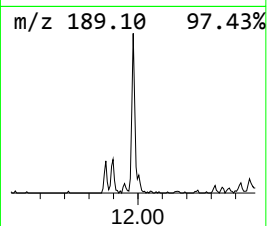
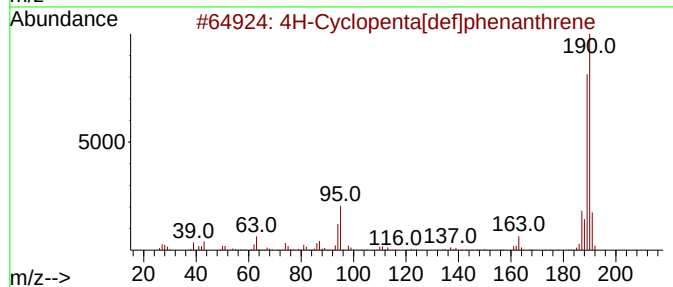
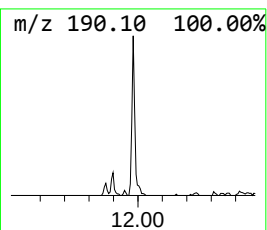
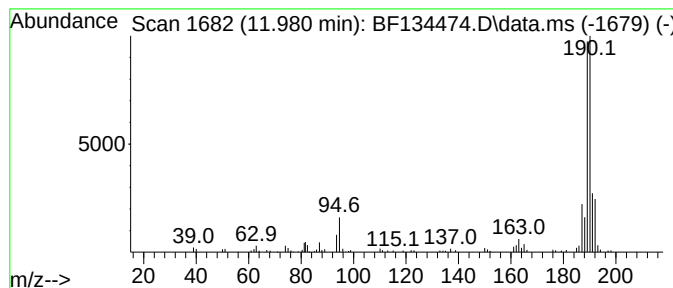
Instrument :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.980	2.60 ng	75936	Phenanthrene-d10	11.363	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	89
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	59
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	36
5	Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	27



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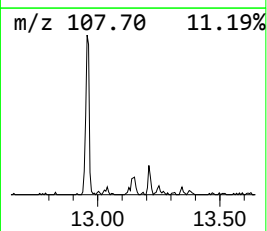
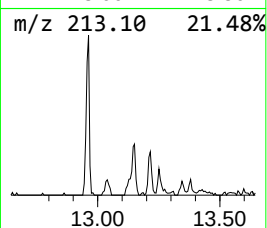
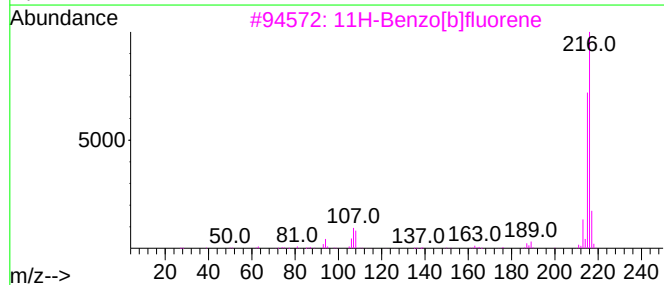
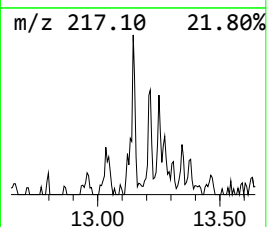
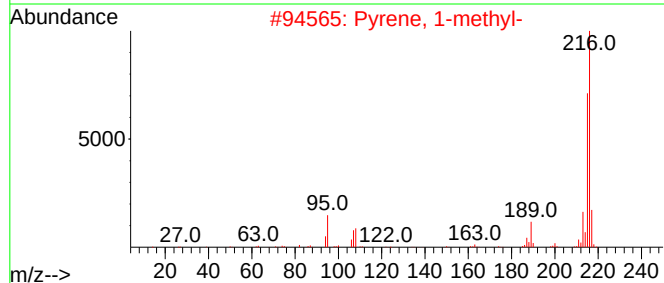
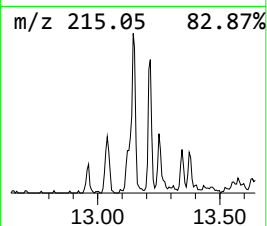
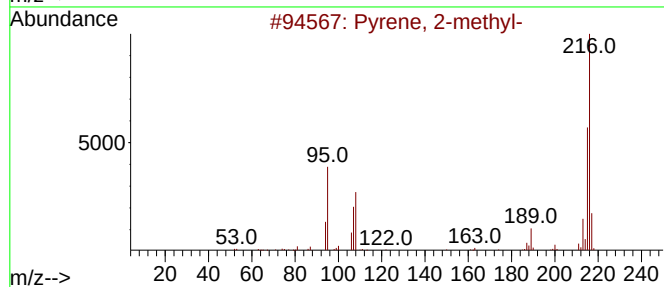
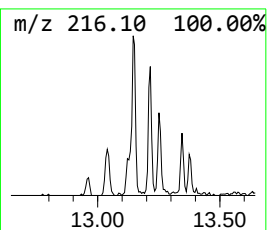
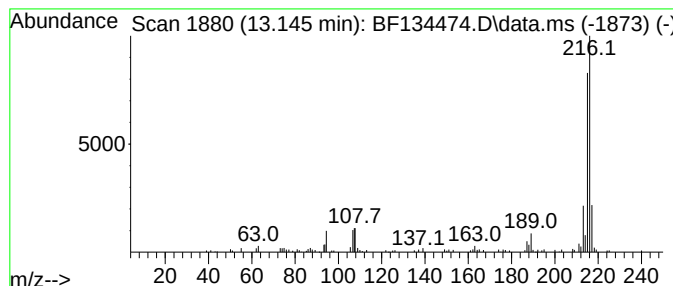
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Pyrene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.145	2.35 ng	98675	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene, 2-methyl-	216	C17H12	003442-78-2	94
2			Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
3			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
4			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
5			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	90



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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
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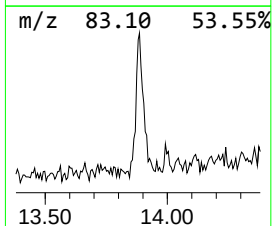
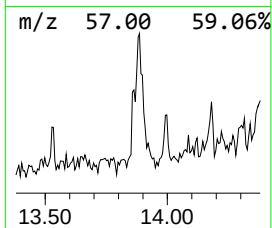
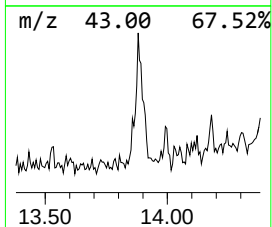
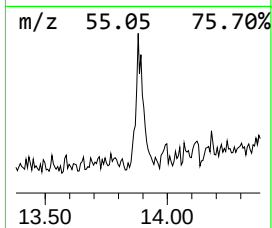
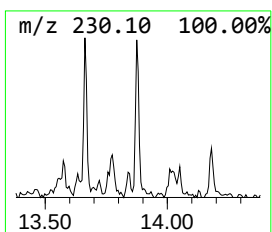
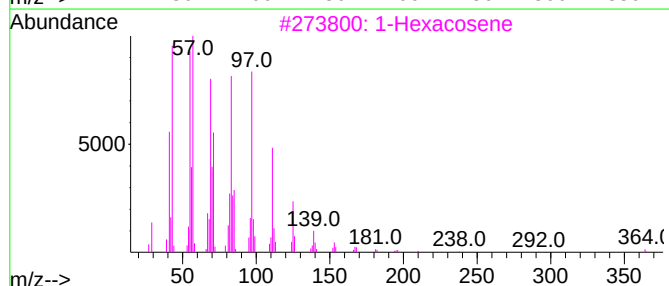
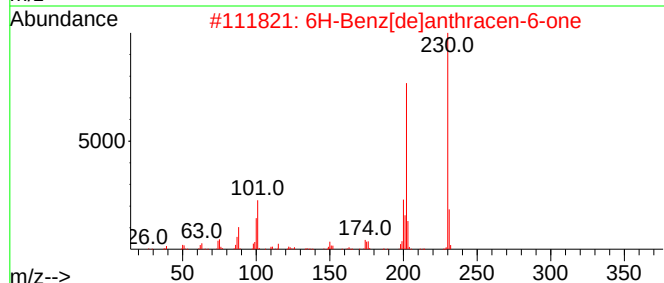
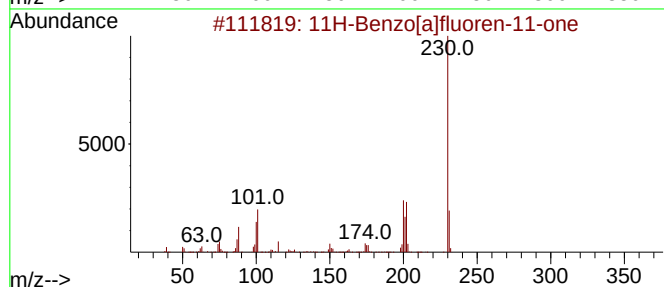
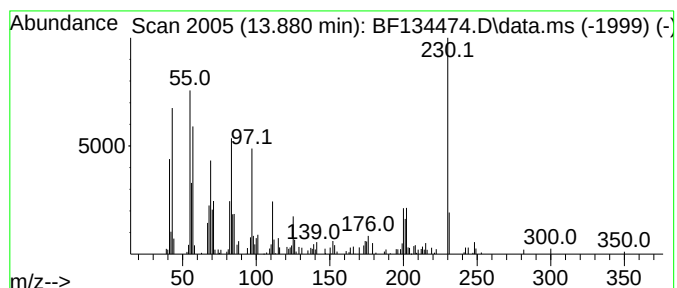
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 11H-Benzo[a]fluoren-11-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	3.54 ng	148702	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	89
2			6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	45
3			1-Hexacosene	364	C26H52	018835-33-1	38
4			1-Eicosanol	298	C20H42O	000629-96-9	38
5			Eicosyl methyl ether	312	C21H44O	1000406-29-4	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072523\
Data File : BF134474.D
Acq On : 25 Jul 2023 21:23
Operator : CG\JU
Sample : 03654-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12016

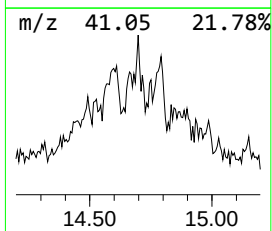
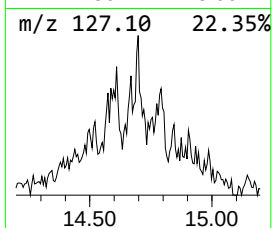
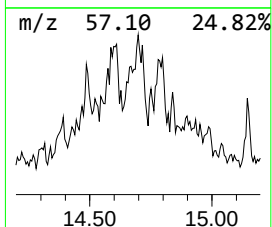
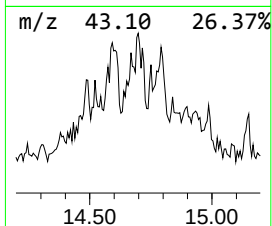
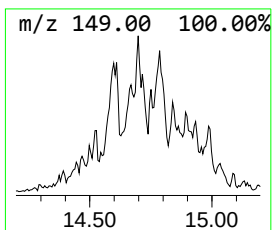
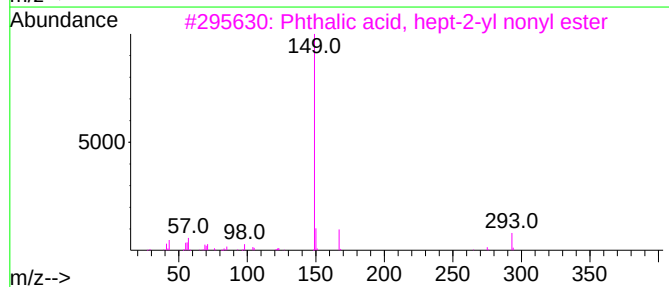
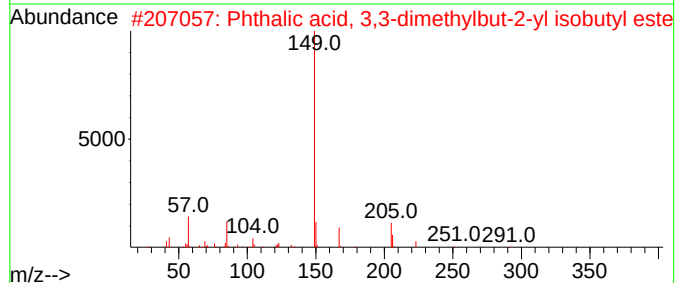
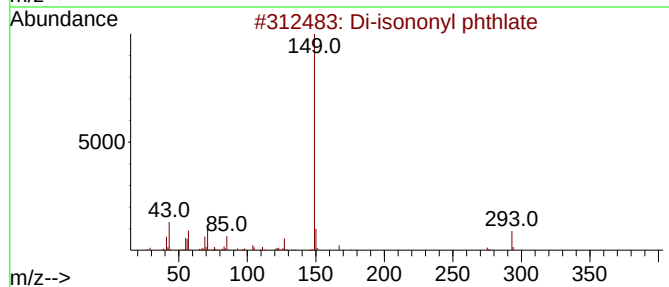
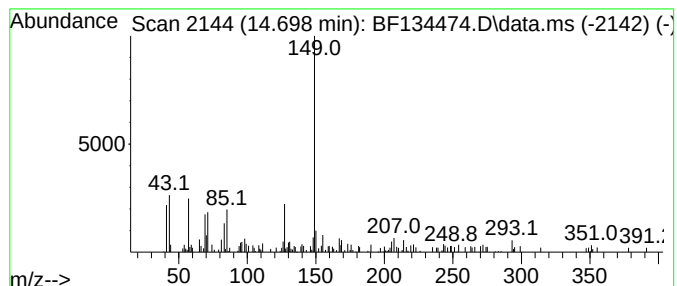
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Di-isononyl phthlate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.698	2.22 ng	93394	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-isononyl phthlate	418	C26H42O4	020548-62-3	50
2			Phthalic acid, 3,3-dimethylbut-2...	306	C18H26O4	1000357-00-1	50
3			Phthalic acid, hept-2-yl nonyl e...	390	C24H38O4	1000356-97-6	47
4			Phthalic acid, hept-4-yl nonyl e...	390	C24H38O4	1000356-79-0	47
5			Phthalic acid, neopentyl pentyl ...	306	C18H26O4	1000315-29-8	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072523\
Data File : BF134474.D
Acq On : 25 Jul 2023 21:23
Operator : CG\JU
Sample : 03654-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12016

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.175	8.8	ng	294019	1	6.834	666482	20.0
n-Hexadecanoic ...	11.892	4.9	ng	143404	4	11.363	585059	20.0
4H-Cyclopenta[d...]	11.980	2.6	ng	75936	4	11.363	585059	20.0
Pyrene, 2-methyl-	13.145	2.4	ng	98675	5	14.027	840595	20.0
11H-Benzo[a]flu...	13.880	3.5	ng	148702	5	14.027	840595	20.0
Di-isononyl pht...	14.698	2.2	ng	93394	5	14.027	840595	20.0