

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
 Data File : BF134363.D
 Acq On : 19 Jul 2023 17:30
 Operator : CG\JU
 Sample : 03597-14
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RB-48-(2-5)

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: BF134363.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	13	rVB	366976	462818	26.88%	3.635%
2	5.087	506	510	520	rVB	24206	31889	1.85%	0.250%
3	5.475	572	576	594	rBV	1459702	1393496	80.93%	10.943%
4	6.481	742	747	767	rBV	1513453	1429397	83.01%	11.225%
5	6.840	804	808	817	rBV	407770	375659	21.82%	2.950%
6	7.398	899	903	915	rBV	925327	921137	53.50%	7.234%
7	8.116	1021	1025	1028	rBV	623144	481253	27.95%	3.779%
8	9.192	1204	1208	1211	rBV	2254383	1721874	100.00%	13.522%
9	9.875	1320	1324	1327	rBV	597419	495269	28.76%	3.889%
10	10.669	1455	1459	1474	rBV	1176115	1020284	59.25%	8.013%
11	11.369	1574	1578	1580	rBV	555621	450018	26.14%	3.534%
12	11.392	1580	1582	1587	rVV	152178	126423	7.34%	0.993%
13	11.433	1587	1589	1594	rVB2	17526	22579	1.31%	0.177%
14	11.898	1665	1668	1675	rBV2	163382	151197	8.78%	1.187%
15	12.592	1782	1786	1789	rBV	199321	179238	10.41%	1.408%
16	12.686	1800	1802	1808	rBV2	28455	34345	1.99%	0.270%
17	12.822	1819	1825	1829	rVB	157398	158931	9.23%	1.248%
18	12.963	1842	1849	1853	rBV	1554708	1452030	84.33%	11.403%
19	13.151	1878	1881	1884	rVB	21290	23737	1.38%	0.186%
20	13.669	1965	1969	1974	rVB	22199	23116	1.34%	0.182%
21	13.774	1984	1987	1990	rBV	21245	22363	1.30%	0.176%
22	13.892	2001	2007	2022	rVB6	67431	191981	11.15%	1.508%
23	14.027	2022	2030	2033	rBV2	406879	480846	27.93%	3.776%
24	14.057	2033	2035	2041	rVB	97748	86876	5.05%	0.682%
25	14.121	2042	2046	2050	rVB2	38520	41172	2.39%	0.323%
26	14.186	2054	2057	2063	rBV3	26674	30786	1.79%	0.242%
27	14.498	2107	2110	2115	rVB5	27123	31088	1.81%	0.244%
28	14.545	2115	2118	2121	rBV4	23425	33106	1.92%	0.260%
29	15.092	2207	2211	2214	rBV	73569	104266	6.06%	0.819%
30	15.157	2219	2222	2227	rVB2	39621	48480	2.82%	0.381%
31	15.239	2234	2236	2243	rBV7	11860	22600	1.31%	0.177%
32	15.404	2260	2264	2270	rVB	38195	60847	3.53%	0.478%
33	15.468	2272	2275	2281	rVB	50912	64371	3.74%	0.506%
34	15.533	2281	2286	2296	rBV	215856	327827	19.04%	2.575%
35	15.768	2322	2326	2332	rVB8	26142	38357	2.23%	0.301%
36	16.010	2363	2367	2372	rBV	28873	44000	2.56%	0.346%

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RB-48-(2-5)

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	16.145	2384	2390	2393	rBV8	17248	38479	2.23%	0.302%
38	16.857	2508	2511	2521	rVB8	11817	23481	1.36%	0.184%
39	17.080	2545	2549	2556	rVB2	24868	53386	3.10%	0.419%
40	17.545	2623	2628	2637	rBV4	14876	34613	2.01%	0.272%

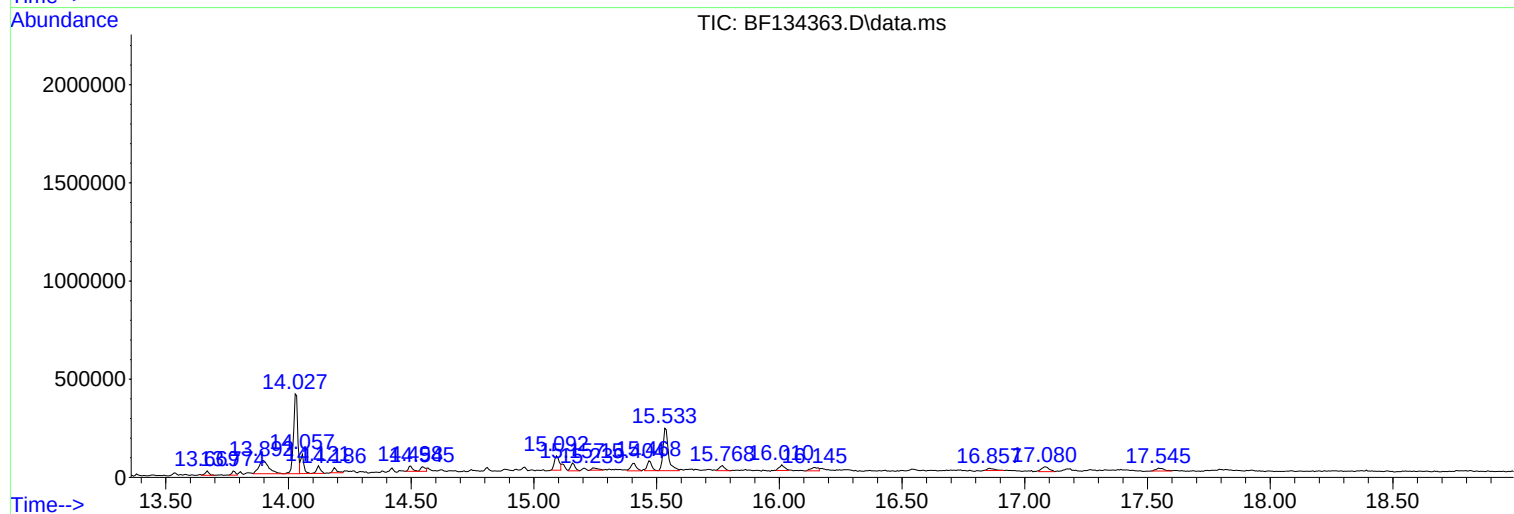
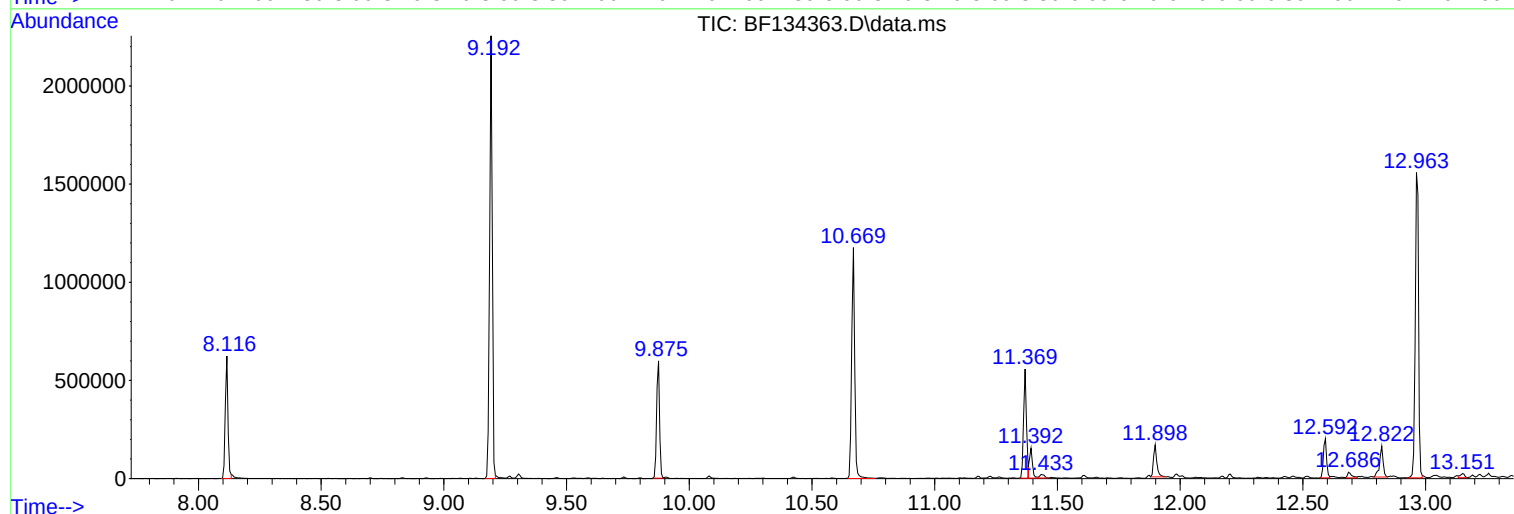
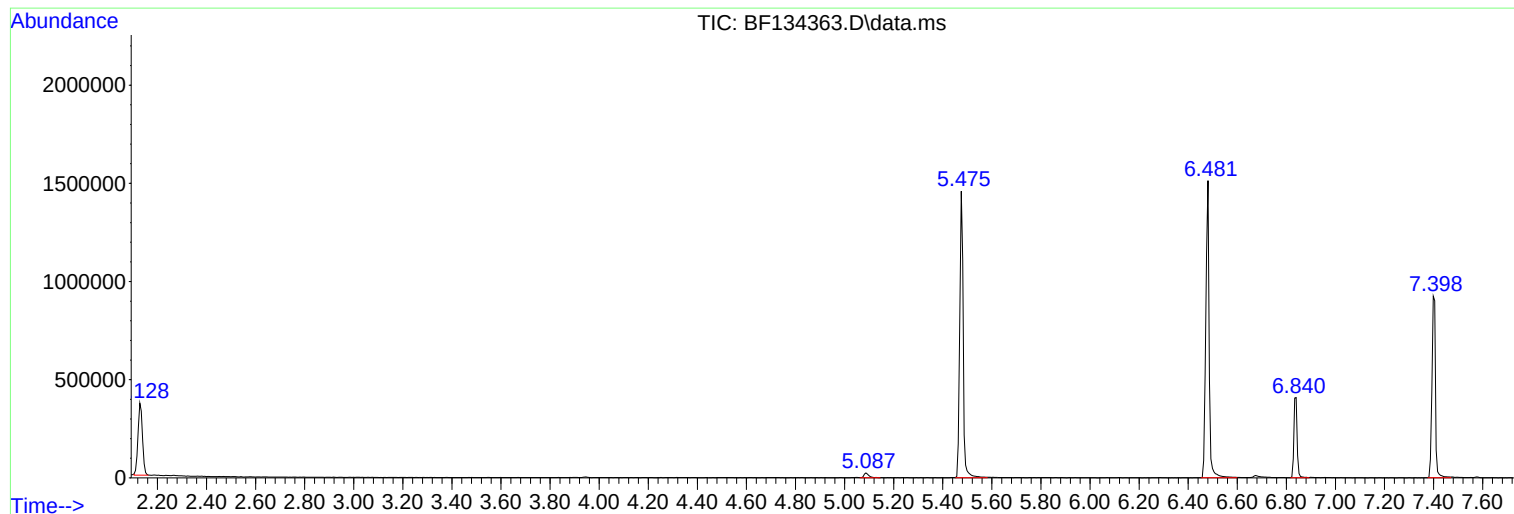
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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RB-48-(2-5)

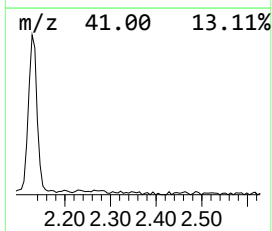
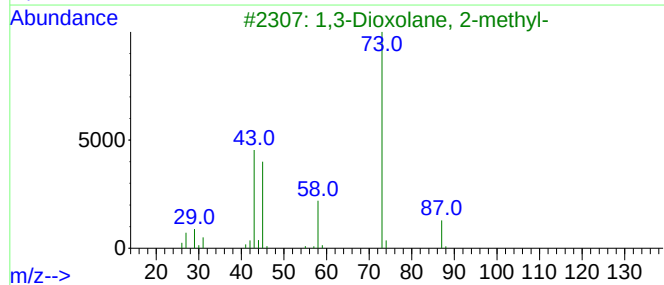
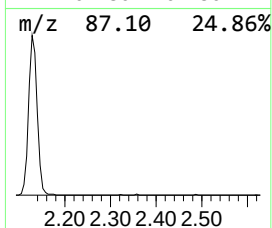
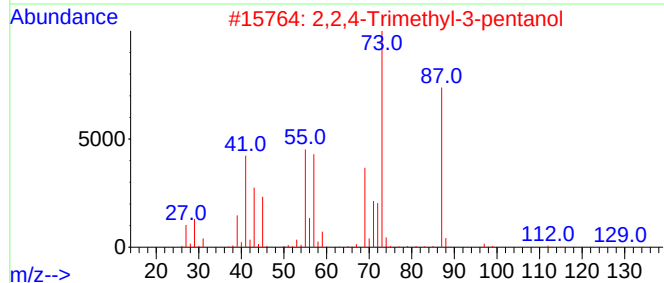
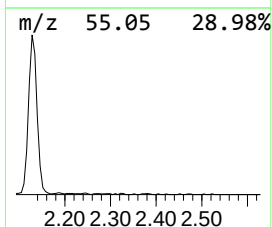
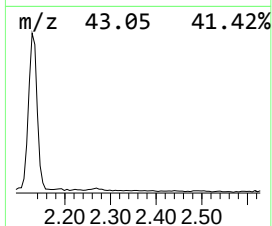
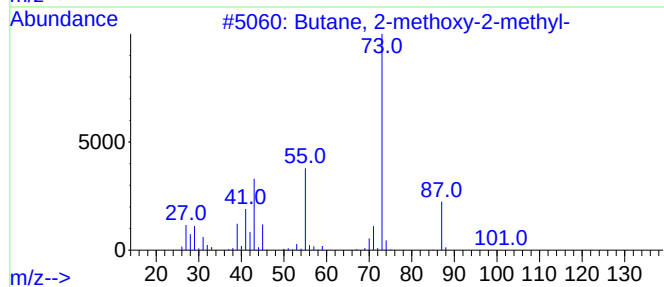
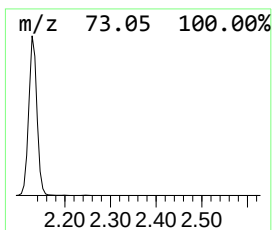
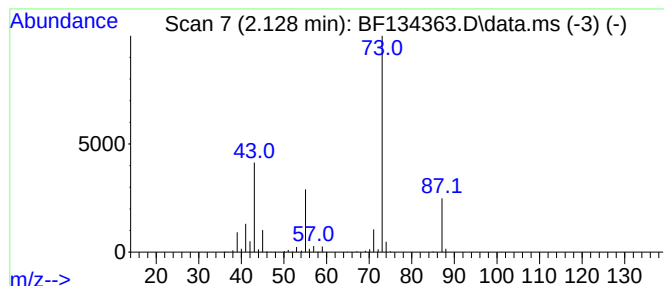
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	24.64 ng	462818	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17



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Instrument :
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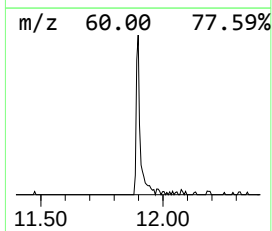
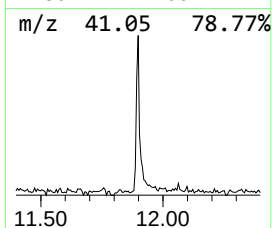
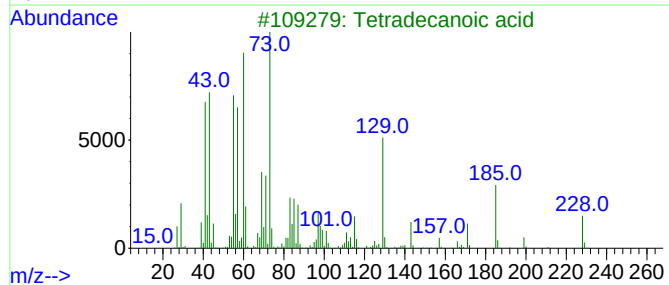
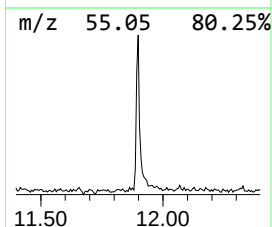
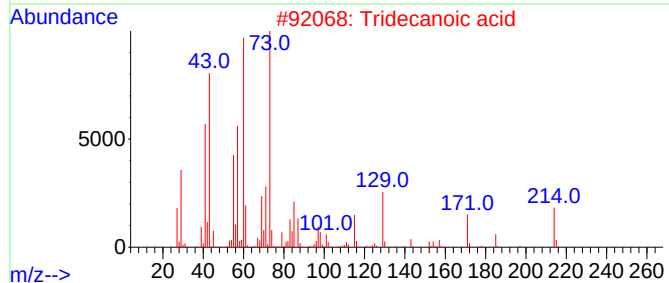
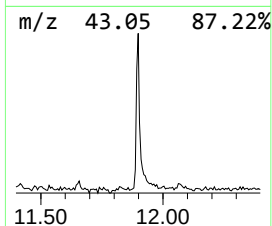
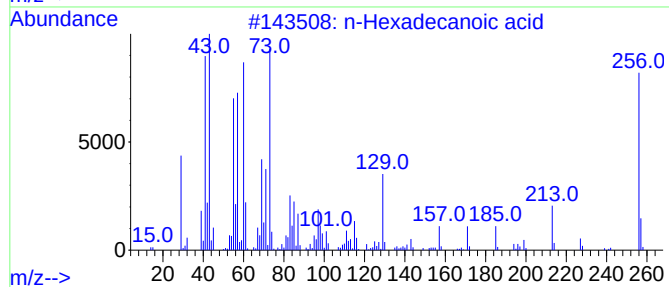
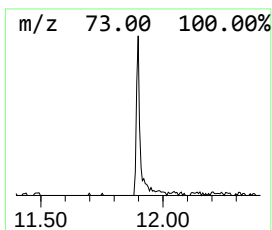
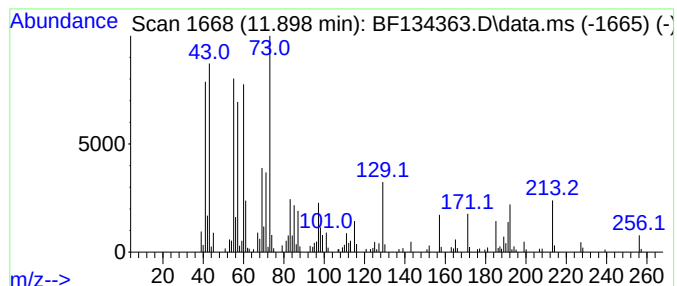
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	6.72 ng	151197	Phenanthrene-d10	11.369

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
2			Tridecanoic acid	214	C13H26O2	000638-53-9	64
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5			Lactose	342	C12H22O11	000063-42-3	47



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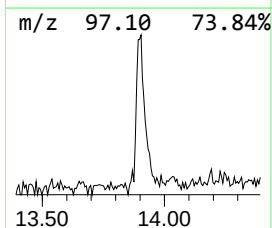
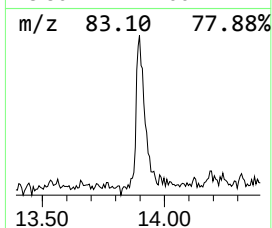
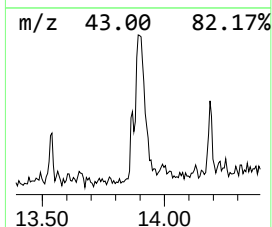
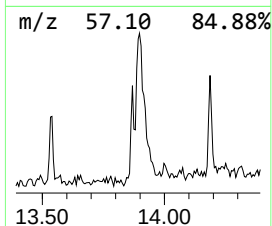
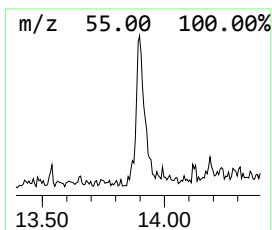
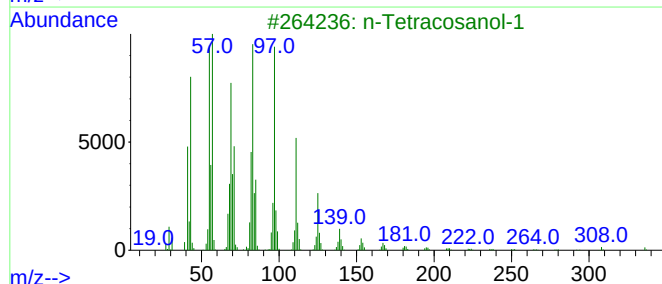
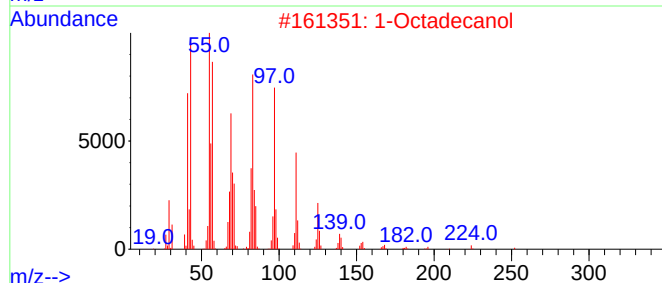
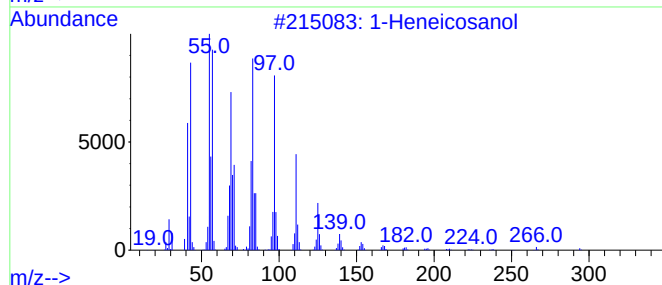
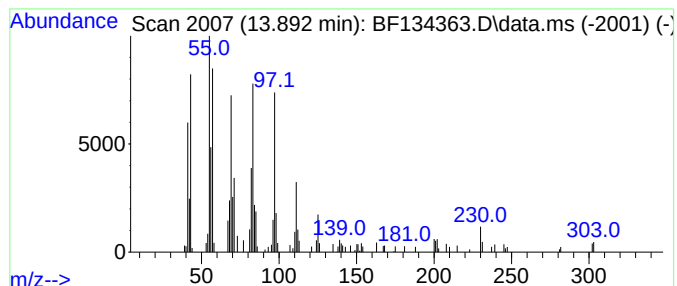
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.892	7.99 ng	191981	Chrysene-d12	14.033	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	1-Octadecanol	270	C18H38O	000112-92-5	90
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	87
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	87
5	Behenic alcohol	326	C22H46O	000661-19-8	87



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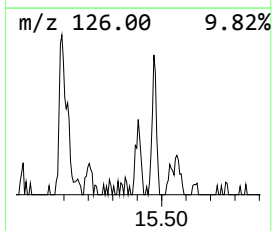
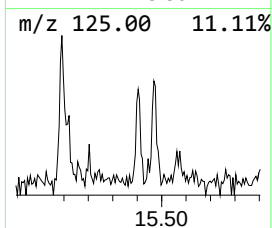
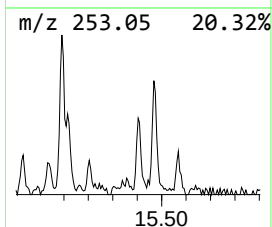
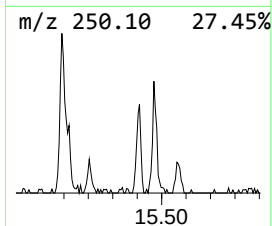
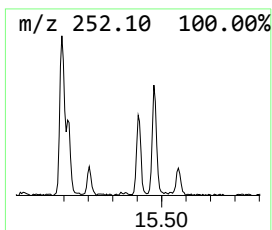
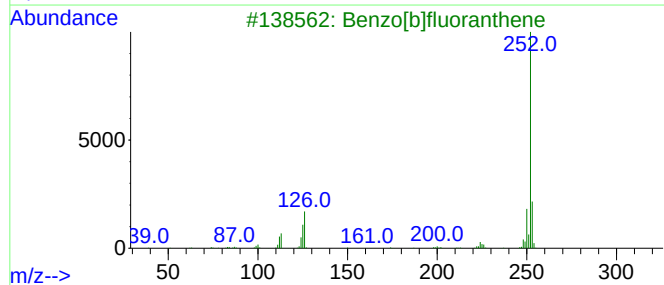
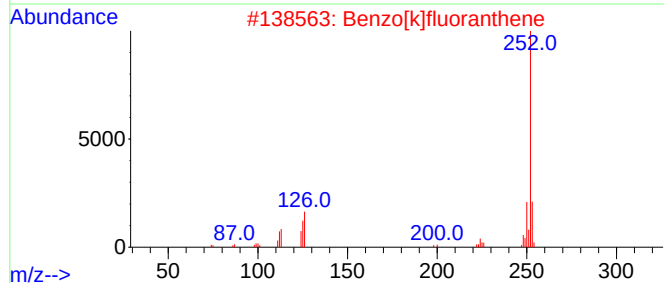
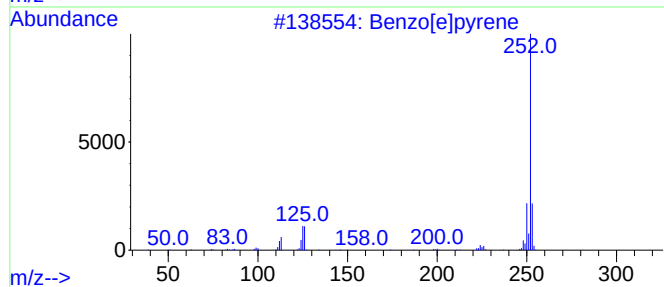
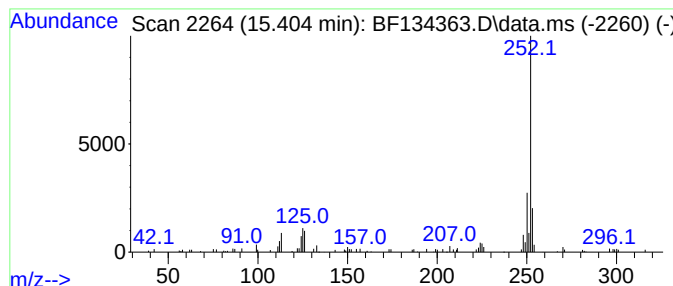
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.404	3.71 ng	60847	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	97
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4			Benzo[a]pyrene	252	C20H12	000050-32-8	87
5			Perylene	252	C20H12	000198-55-0	86



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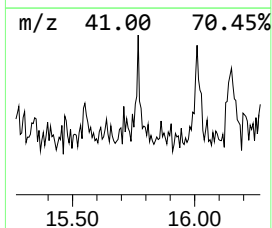
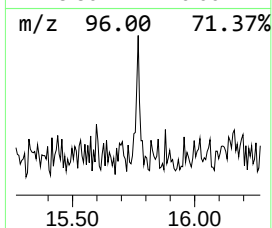
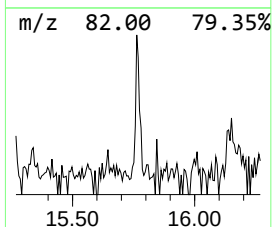
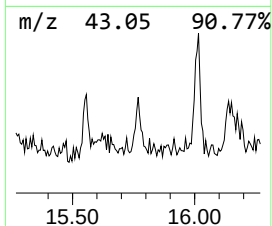
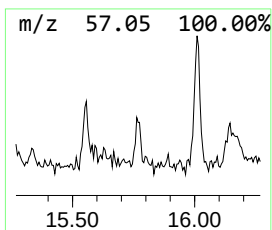
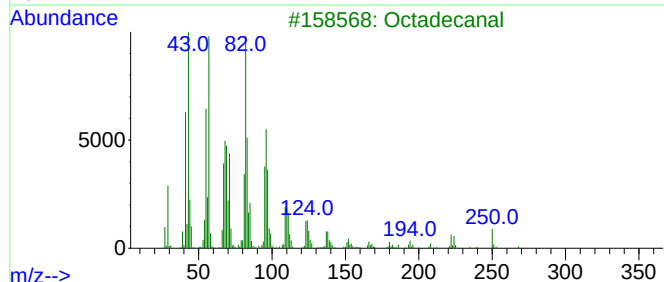
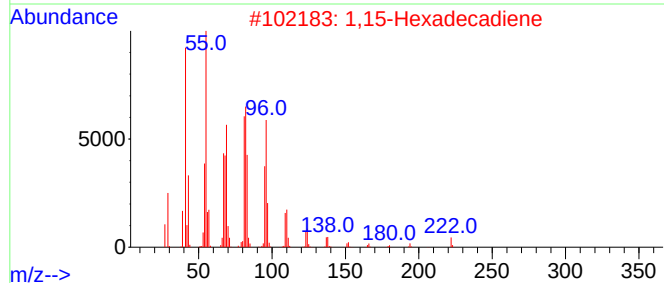
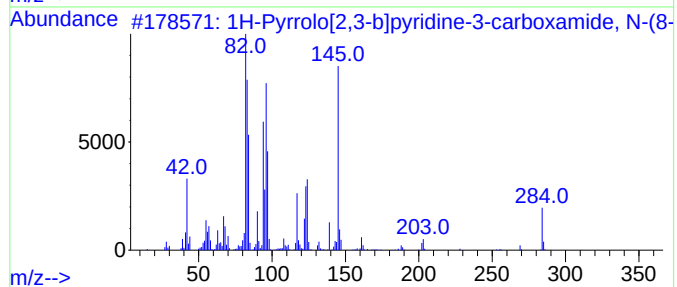
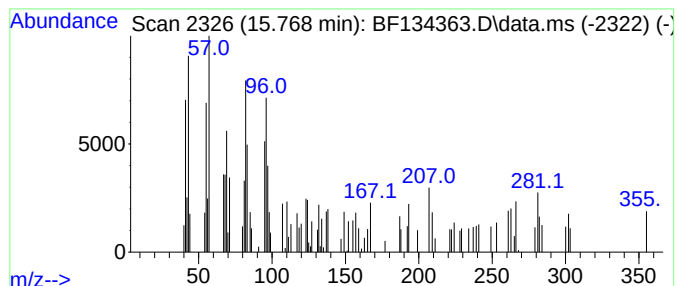
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1H-Pyrrolo[2,3-b]pyridine-3... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.768	2.34 ng	38357	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Pyrrolo[2,3-b]pyridine-3-carb...	284	C16H20N4O	1955758-70-9	90
2			1,15-Hexadecadiene	222	C16H30	021964-51-2	78
3			Octadecanal	268	C18H36O	000638-66-4	60
4			Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	49
5			E-11(13-Methyl)tetradecen-1-ol a...	268	C17H32O2	1000130-80-4	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
Data File : BF134363.D
Acq On : 19 Jul 2023 17:30
Operator : CG\JU
Sample : 03597-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-48-(2-5)

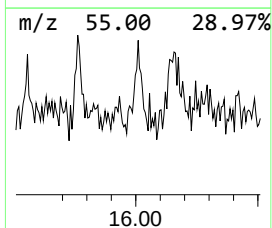
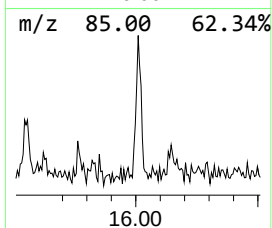
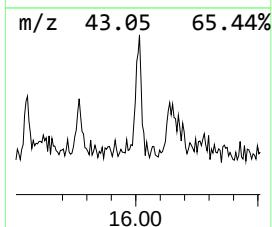
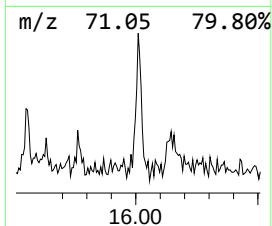
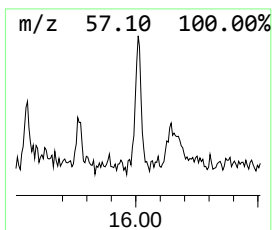
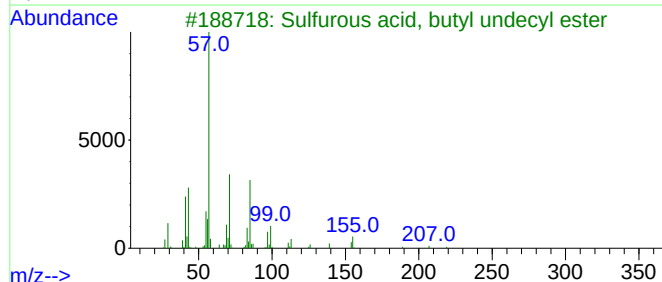
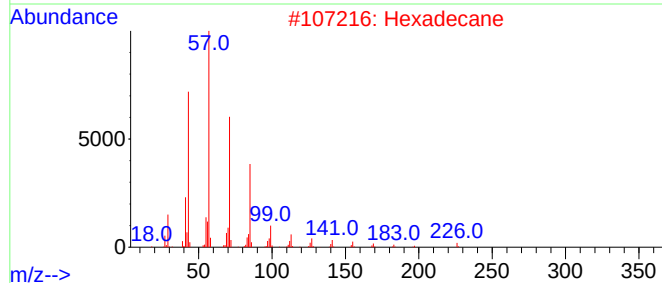
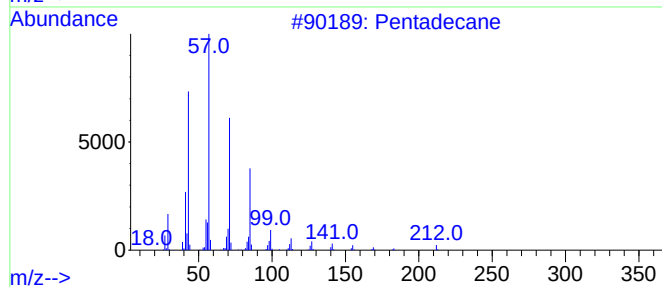
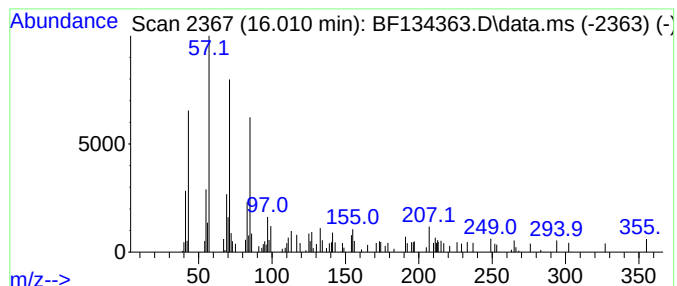
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.010	2.68 ng	44000	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane	212	C15H32	000629-62-9	76
2			Hexadecane	226	C16H34	000544-76-3	76
3			Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	64
4			Heptadecane, 8-methyl-	254	C18H38	013287-23-5	64
5			Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
Data File : BF134363.D
Acq On : 19 Jul 2023 17:30
Operator : CG\JU
Sample : 03597-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
RB-48-(2-5)

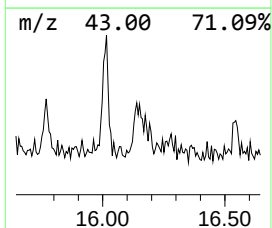
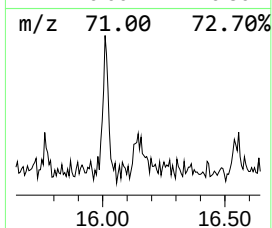
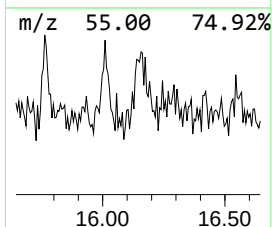
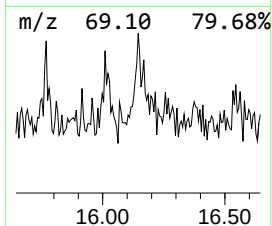
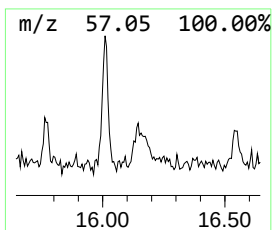
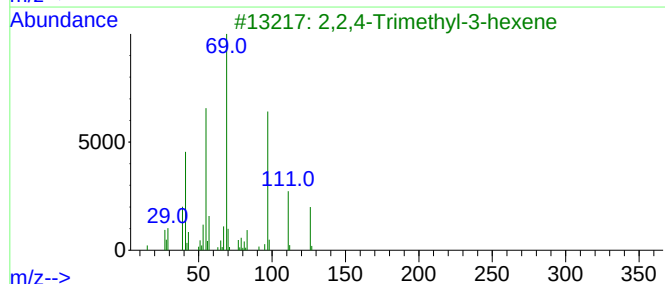
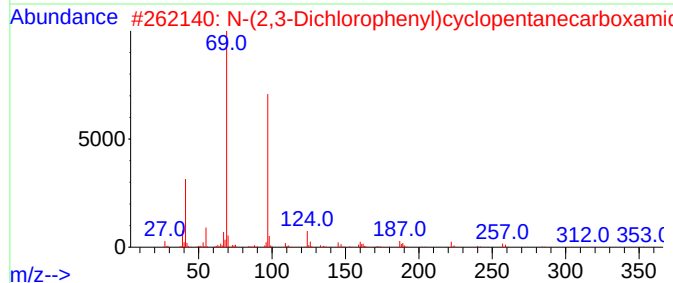
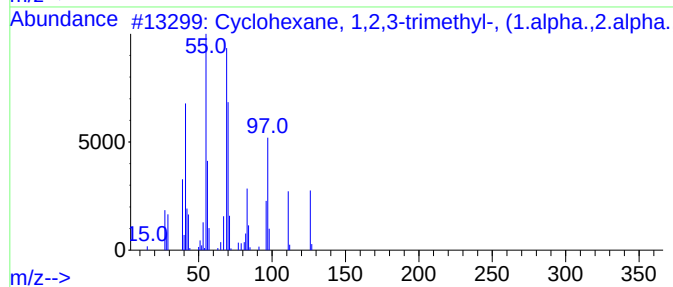
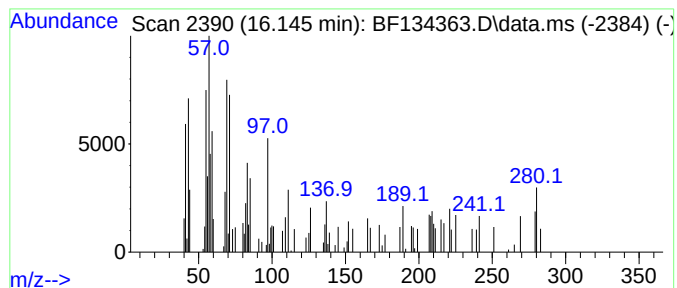
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown16.145 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.145	2.35 ng	38479	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,2,3-trimethyl-, (...	126	C9H18	007667-55-2	41
2			N-(2,3-Dichlorophenyl)cyclopenta...	353	C14H12Cl2F3N02	1000511-05-0	38
3			2,2,4-Trimethyl-3-hexene	126	C9H18	059643-72-0	38
4			2-Methyl-Z-4-tetradecene	210	C15H30	1000130-78-3	38
5			1,2-Dodecanediol	202	C12H26O2	001119-87-5	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
Data File : BF134363.D
Acq On : 19 Jul 2023 17:30
Operator : CG\JU
Sample : 03597-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-48-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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
Butane, 2-metho...	2.128	24.6	ng	462818	1	6.840	375659	20.0
n-Hexadecanoic ...	11.898	6.7	ng	151197	4	11.369	450018	20.0
1-Heneicosanol	13.892	8.0	ng	191981	5	14.033	480846	20.0
Benzo[e]pyrene	15.404	3.7	ng	60847	6	15.533	327827	20.0
1H-Pyrrolo[2,3-...	15.768	2.3	ng	38357	6	15.533	327827	20.0
Pentadecane	16.010	2.7	ng	44000	6	15.533	327827	20.0
unknown16.145	16.145	2.4	ng	38479	6	15.533	327827	20.0