

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
 Data File : BF123599.D
 Acq On : 16 Apr 2021 19:07
 Operator : JU/CG
 Sample : M1967-04
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SED-1B

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-BF041521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123599.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	6	15	22	rVB	2780013	3539864	48.85%	6.264%
2	5.098	509	512	519	rVB	61156	79328	1.09%	0.140%
3	5.487	573	578	581	rBV	7035631	7005893	96.67%	12.397%
4	6.492	743	749	752	rBV	6070107	7246896	100.00%	12.823%
5	6.869	809	813	816	rBV	2065878	1764251	24.34%	3.122%
6	7.428	902	908	911	rBV	4771480	4752117	65.57%	8.409%
7	8.151	1026	1031	1034	rBV	2805916	2325347	32.09%	4.115%
8	9.233	1209	1215	1218	rBV	7563133	6528432	90.09%	11.552%
9	9.622	1278	1281	1285	rBV	277206	223947	3.09%	0.396%
10	9.910	1326	1330	1334	rVB	2733081	2469777	34.08%	4.370%
11	10.704	1459	1465	1468	rBV	5615785	5039817	69.54%	8.918%
12	11.404	1580	1584	1586	rBV	2938219	2584850	35.67%	4.574%
13	11.422	1586	1587	1590	rVV	114762	76302	1.05%	0.135%
14	11.469	1590	1595	1599	rVB3	90506	97260	1.34%	0.172%
15	11.933	1670	1674	1685	rBV	684626	727672	10.04%	1.288%
16	12.616	1787	1790	1795	rBV	319112	261711	3.61%	0.463%
17	12.721	1803	1808	1814	rBV2	201343	229150	3.16%	0.405%
18	12.845	1826	1829	1832	rVB	243875	191617	2.64%	0.339%
19	12.892	1835	1837	1845	rVB3	96012	95992	1.32%	0.170%
20	12.998	1850	1855	1858	rVB	5750289	5688926	78.50%	10.067%
21	13.227	1891	1894	1899	rBV2	95525	123287	1.70%	0.218%
22	13.474	1929	1936	1942	rBV6	40693	87562	1.21%	0.155%
23	13.568	1950	1952	1955	rBV	124807	110040	1.52%	0.195%
24	13.904	2005	2009	2010	rBV	257349	243609	3.36%	0.431%
25	14.051	2028	2034	2037	rBV	2171675	2128258	29.37%	3.766%
26	14.216	2060	2062	2067	rVB	168324	157119	2.17%	0.278%
27	14.527	2110	2115	2118	rBV	183040	184858	2.55%	0.327%
28	14.839	2164	2168	2171	rBV	150068	134779	1.86%	0.238%
29	14.915	2178	2181	2188	rBV	79376	86731	1.20%	0.153%
30	15.098	2207	2212	2215	rBV	95692	150286	2.07%	0.266%
31	15.186	2223	2227	2234	rVB2	123340	161957	2.23%	0.287%
32	15.404	2259	2264	2270	rBV2	55081	83192	1.15%	0.147%
33	15.468	2271	2275	2279	rVV	87242	99628	1.37%	0.176%
34	15.533	2281	2286	2290	rVV	1131753	1469853	20.28%	2.601%
35	15.574	2290	2293	2300	rVB2	109754	168675	2.33%	0.298%
36	16.027	2365	2370	2375	rBV	70252	109734	1.51%	0.194%

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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-BF041521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.551	2453	2459	2464	rBV3	44322	83984	1.16%	0.149%
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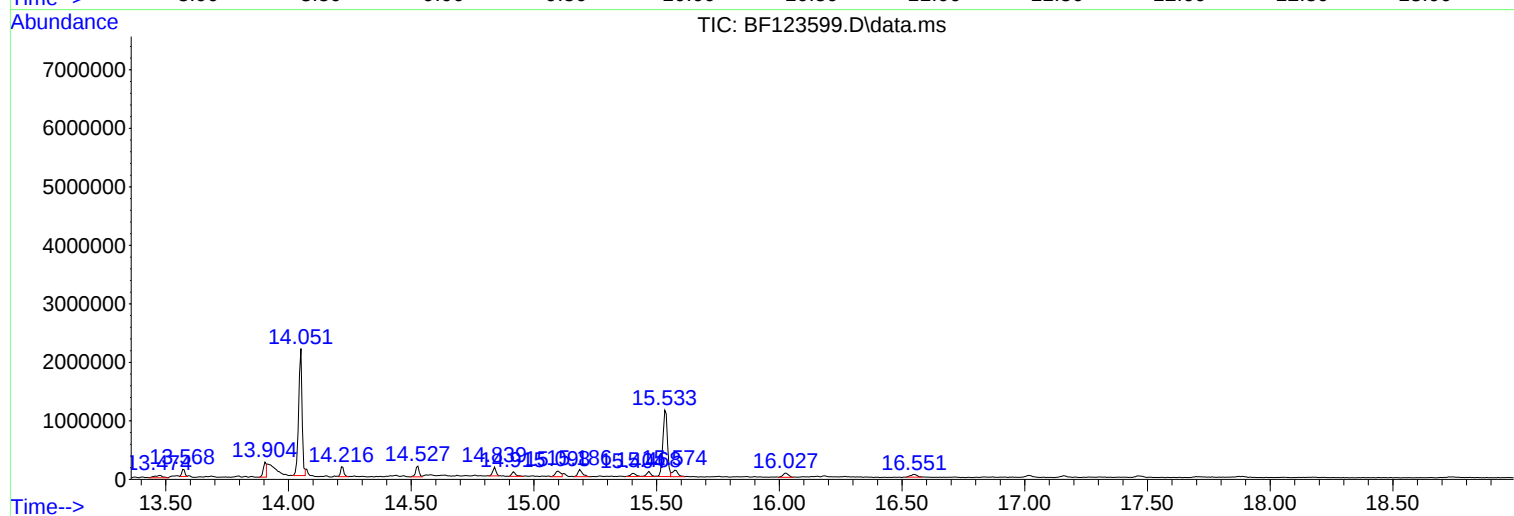
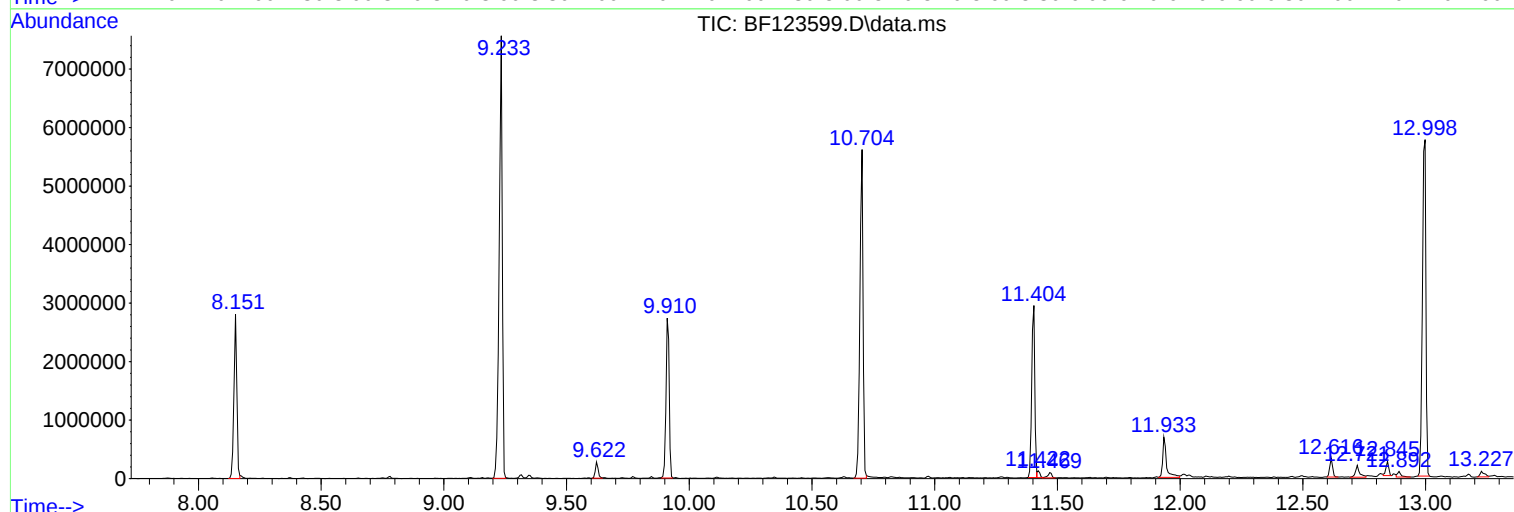
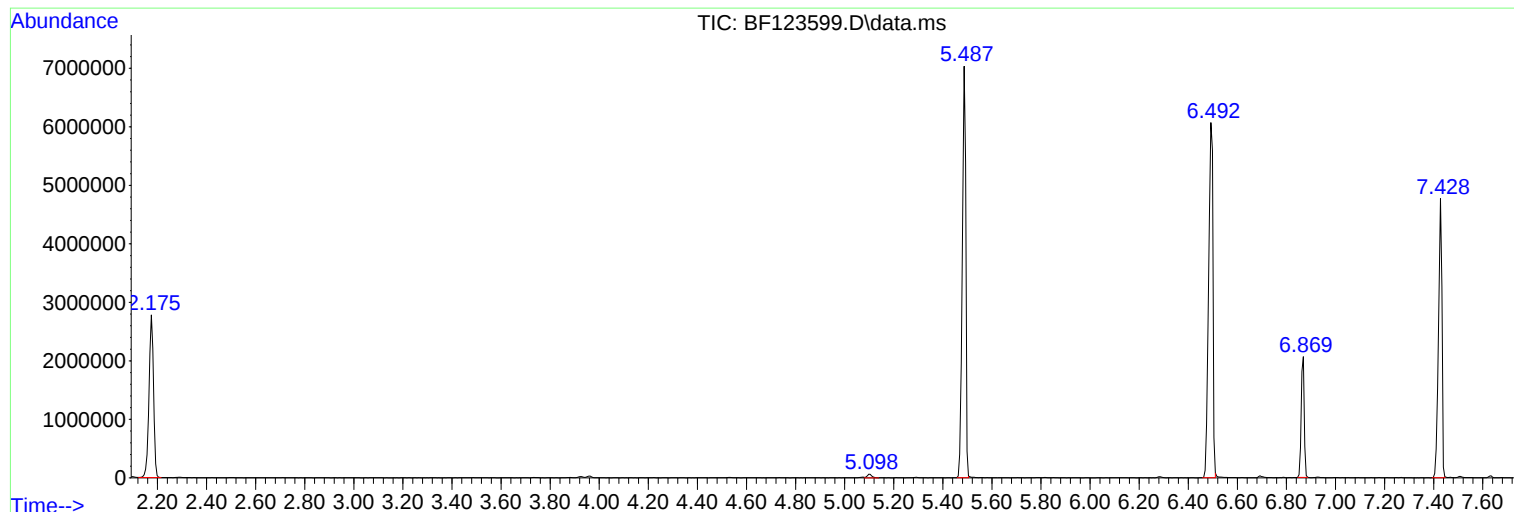
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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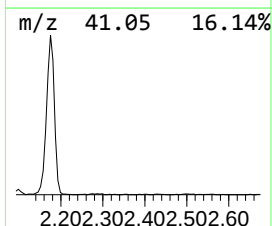
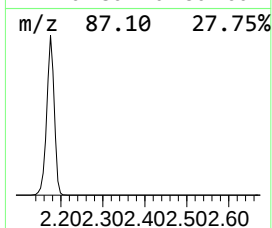
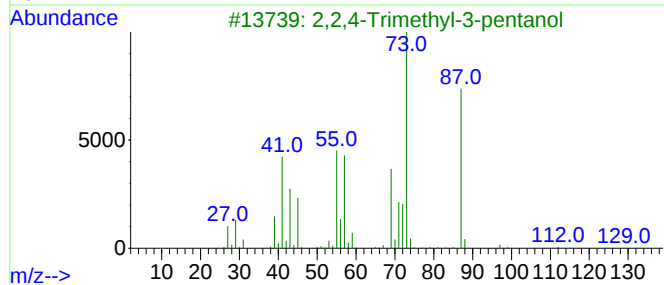
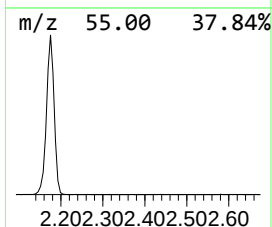
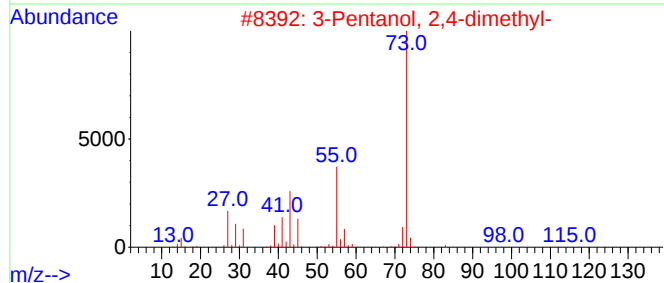
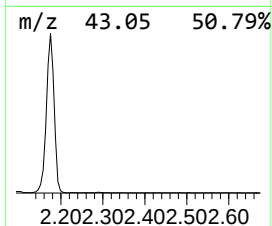
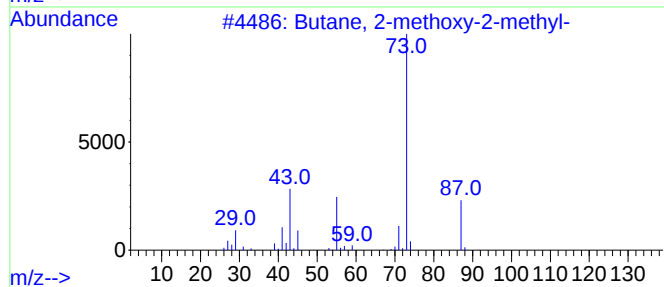
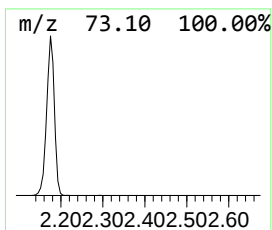
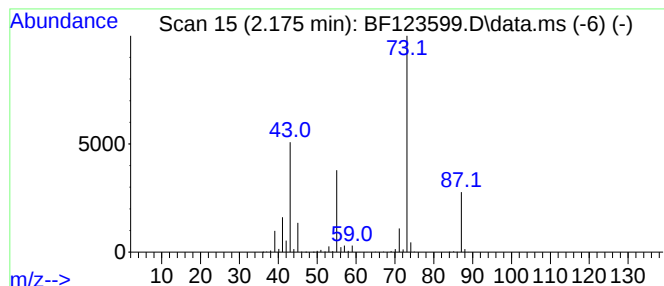
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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	40.13 ng	3539860	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25



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ClientSampleId :
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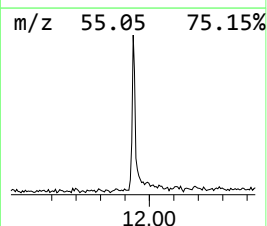
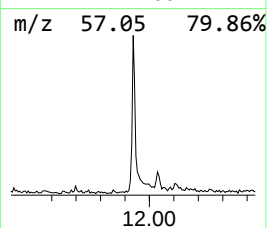
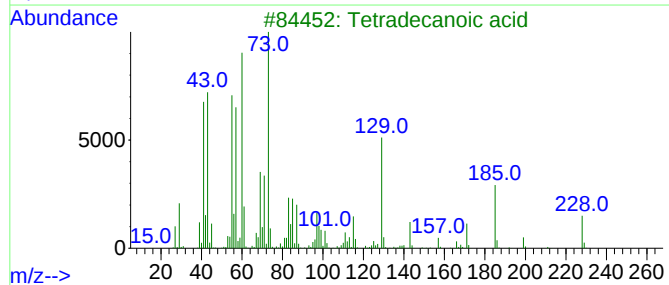
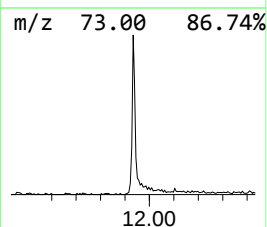
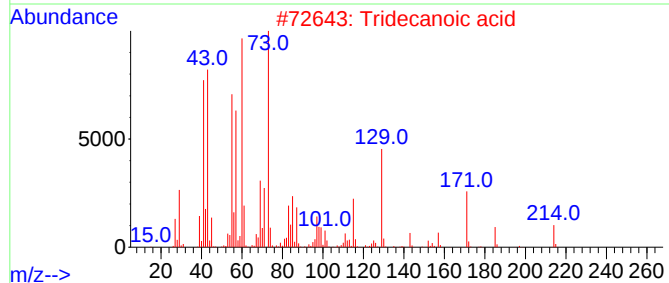
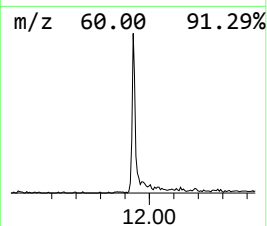
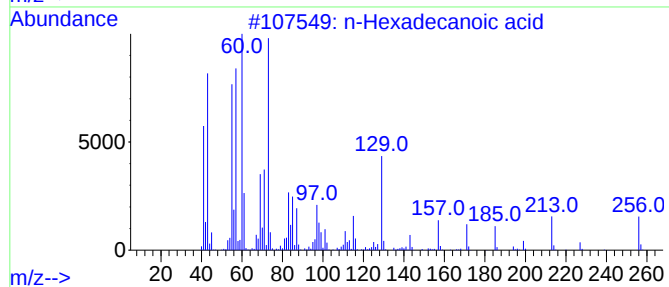
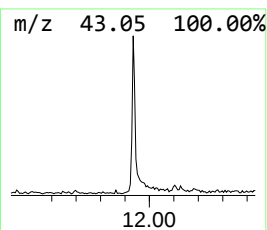
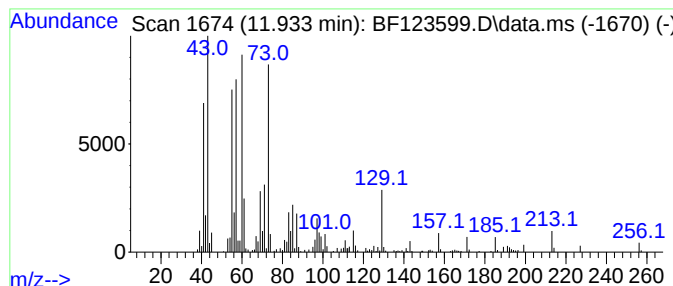
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	5.63 ng	727672	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4			Undecanoic acid	186	C11H22O2	000112-37-8	86
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	47



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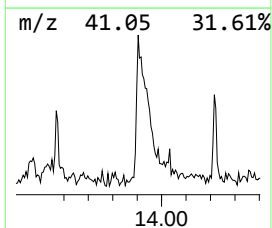
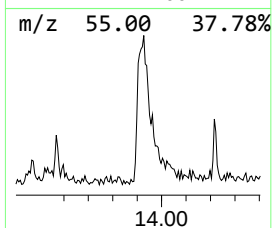
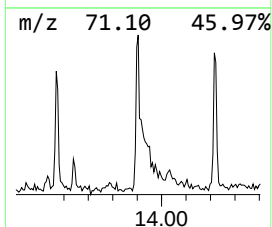
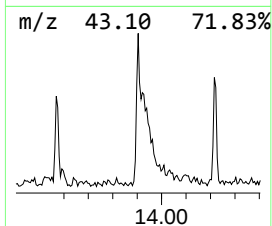
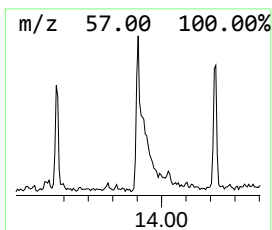
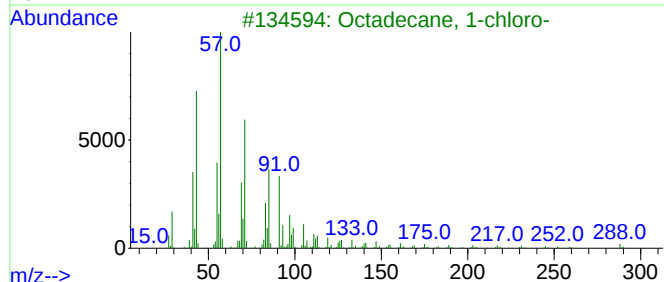
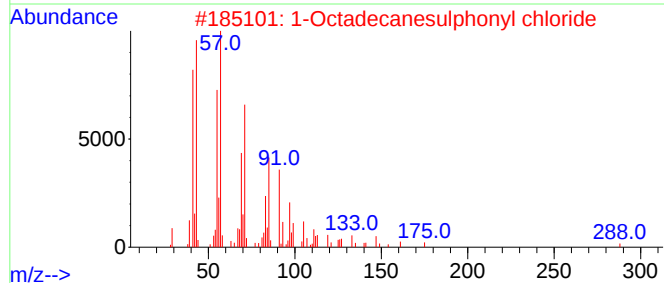
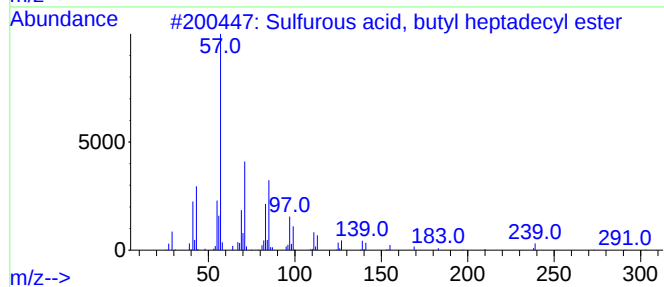
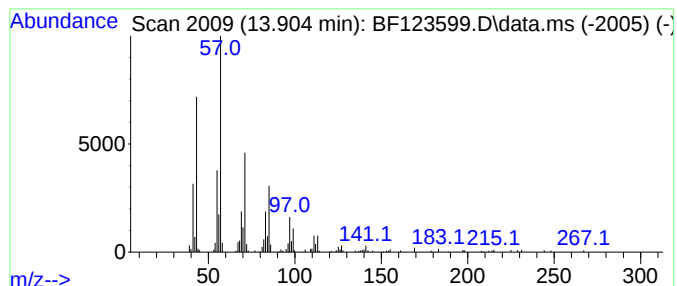
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Sulfurous acid, butyl hepta... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	2.29 ng	243609	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	91
2			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	91
3			Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	91
4			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	87
5			Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	86



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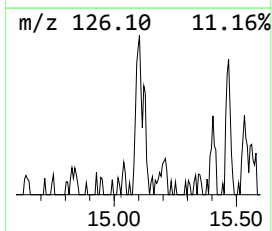
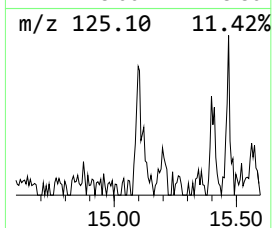
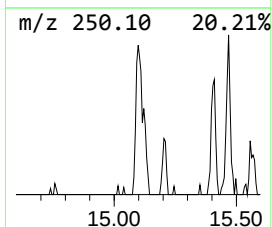
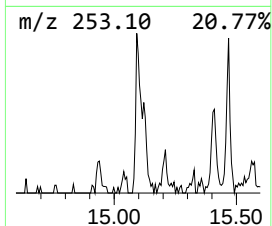
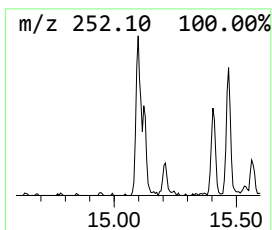
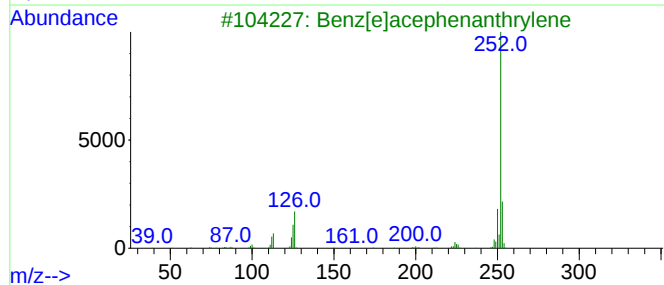
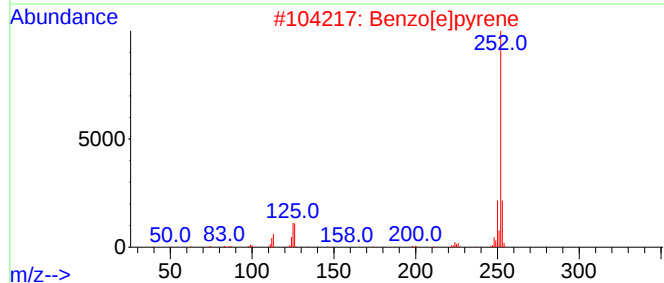
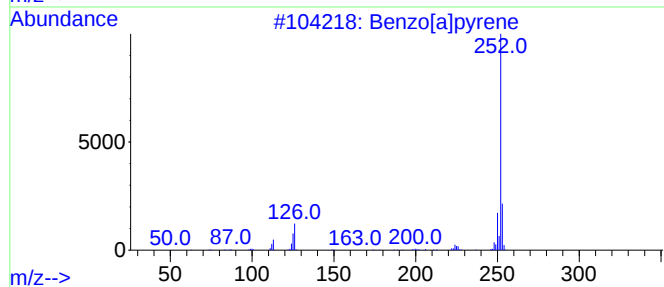
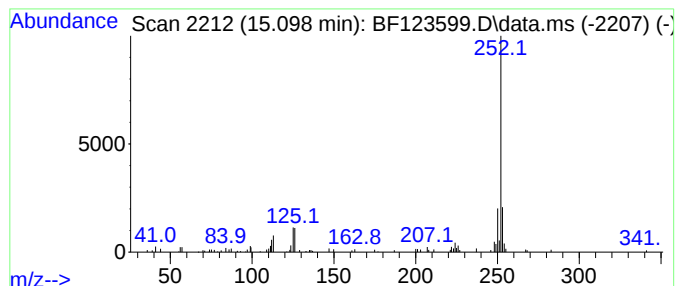
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.098	2.04 ng	150286	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[a]pyrene	252	C20H12	000050-32-8	93
2			Benzo[e]pyrene	252	C20H12	000192-97-2	91
3			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	90
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	89
5			Perylene	252	C20H12	000198-55-0	81



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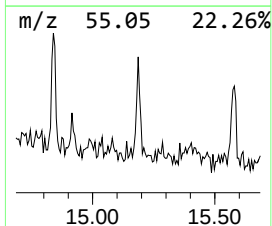
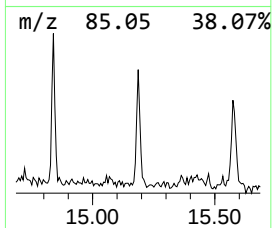
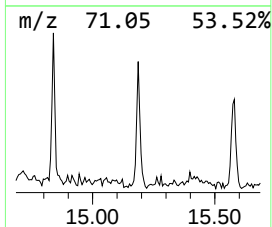
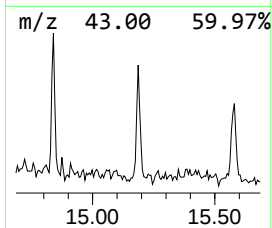
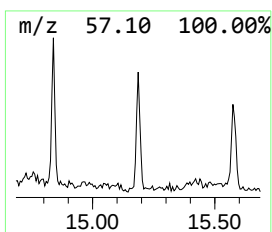
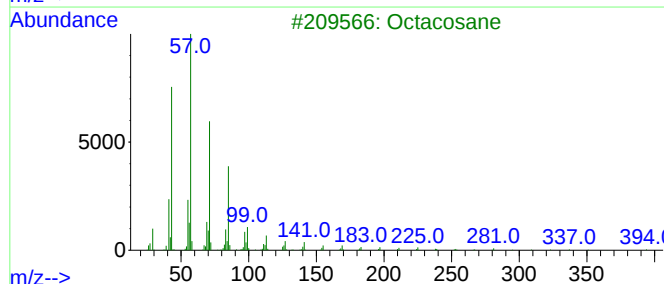
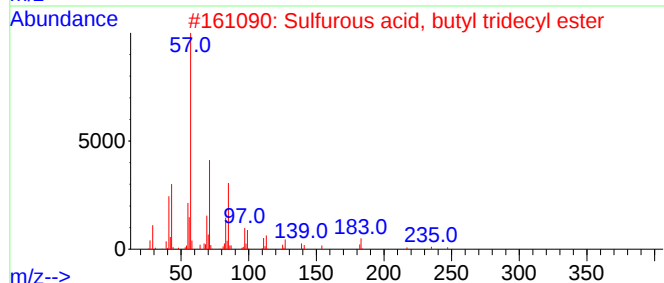
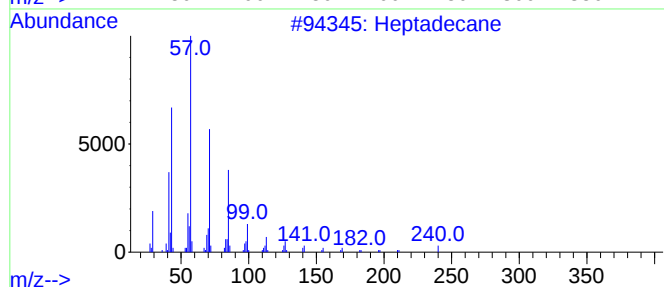
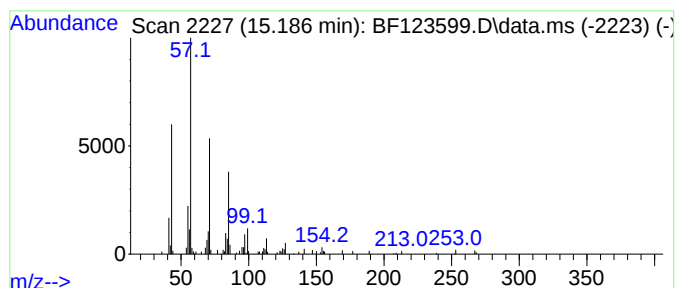
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.186	2.20 ng	161957	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	80
2			Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	78
3			Octacosane	394	C28H58	000630-02-4	78
4			1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	78
5			Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123599.D
Acq On : 16 Apr 2021 19:07
Operator : JU/CG
Sample : M1967-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SED-1B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.175	40.1	ng	3539860	1	6.869	1764250	20.0
n-Hexadecanoic ...	11.933	5.6	ng	727672	4	11.404	2584850	20.0
Sulfurous acid,...	13.904	2.3	ng	243609	5	14.051	2128260	20.0
Benzo[e]pyrene	15.098	2.0	ng	150286	6	15.533	1469850	20.0
Heptadecane	15.186	2.2	ng	161957	6	15.533	1469850	20.0