

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
 Data File : BF124807.D
 Acq On : 27 Jul 2021 22:40
 Operator : JU/CG
 Sample : M3151-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-2

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-BF072221.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124807.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	10	rVB	9751	10501	5.04%	0.769%
2	5.087	507	510	513	rBB	2480	2463	1.18%	0.180%
3	5.481	573	577	581	rBB	121643	122971	58.99%	9.005%
4	6.492	745	749	752	rBV	128173	129172	61.97%	9.459%
5	6.869	810	813	816	rBB	43056	30231	14.50%	2.214%
6	7.433	905	909	911	rBB	103048	86026	41.27%	6.300%
7	8.051	1011	1014	1018	rBB	13087	9251	4.44%	0.677%
8	8.151	1028	1031	1034	rBB	59341	43846	21.03%	3.211%
9	9.227	1210	1214	1217	rBV	207209	166490	79.87%	12.192%
10	9.910	1326	1330	1333	rBB	68648	54581	26.18%	3.997%
11	10.698	1460	1464	1467	rBB	146600	116745	56.01%	8.549%
12	11.398	1579	1583	1585	rBV	67786	59555	28.57%	4.361%
13	11.416	1585	1586	1589	rVB	4531	2638	1.27%	0.193%
14	11.916	1668	1671	1674	rBB	19261	15274	7.33%	1.119%
15	12.486	1765	1768	1770	rBB	3748	2886	1.38%	0.211%
16	12.604	1786	1788	1791	rBB	8822	6953	3.34%	0.509%
17	12.704	1802	1805	1808	rBB	14301	9788	4.70%	0.717%
18	12.833	1825	1827	1831	rBB	7571	7159	3.43%	0.524%
19	12.986	1848	1853	1856	rBV	233786	208451	100.00%	15.265%
20	13.204	1888	1890	1892	rBB	6903	4822	2.31%	0.353%
21	13.551	1946	1949	1951	rBB	13979	12006	5.76%	0.879%
22	13.880	2001	2005	2010	rBV	28394	31752	15.23%	2.325%
23	14.033	2027	2031	2034	rBV	60206	48228	23.14%	3.532%
24	14.192	2055	2058	2061	rBV	33380	24965	11.98%	1.828%
25	14.498	2107	2110	2113	rBB	32832	26808	12.86%	1.963%
26	14.604	2125	2128	2132	rBB	2599	2400	1.15%	0.176%
27	14.721	2144	2148	2152	rVB	7950	8378	4.02%	0.614%
28	14.804	2156	2162	2165	rBB2	28190	31972	15.34%	2.341%
29	15.145	2216	2220	2225	rBB	21379	21414	10.27%	1.568%
30	15.509	2277	2282	2284	rBV	31178	38291	18.37%	2.804%
31	15.533	2284	2286	2290	rVB	13748	12699	6.09%	0.930%
32	15.968	2356	2360	2364	rBB	7565	11080	5.32%	0.811%
33	16.480	2442	2447	2452	rBB	3793	5773	2.77%	0.423%

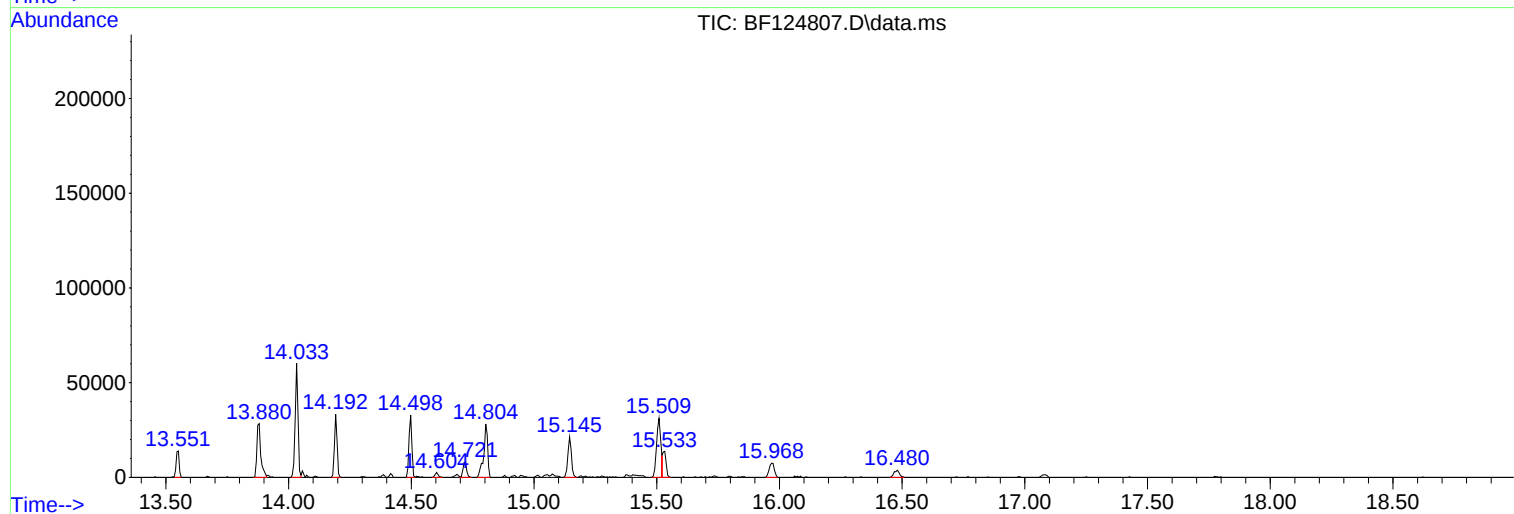
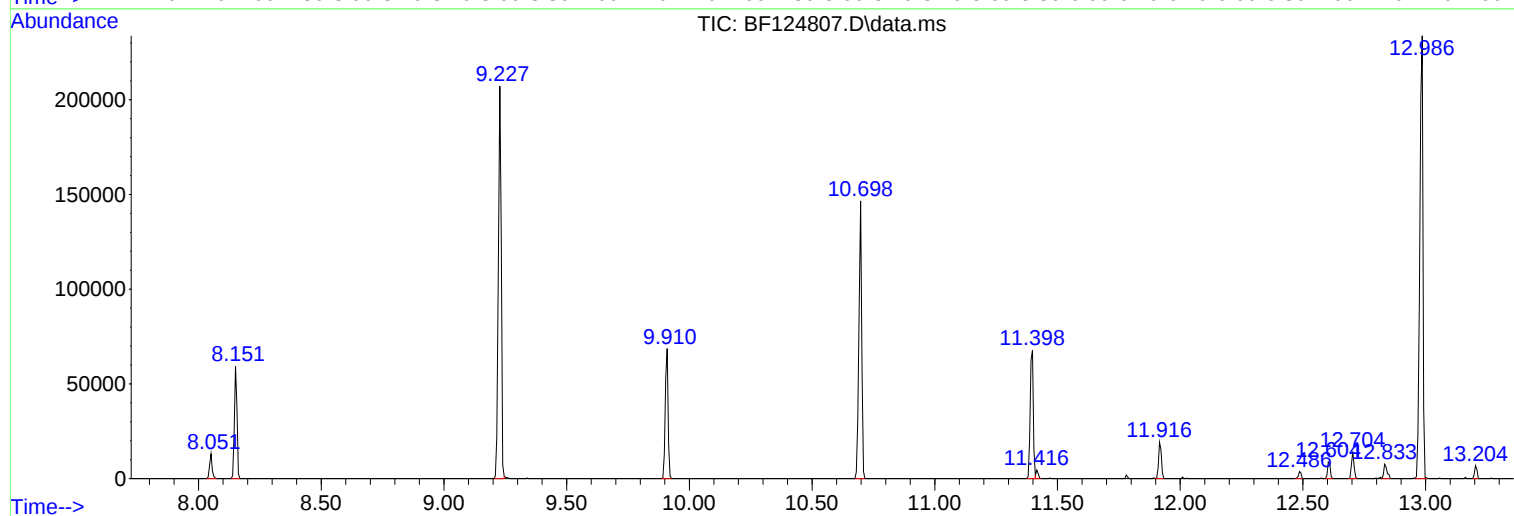
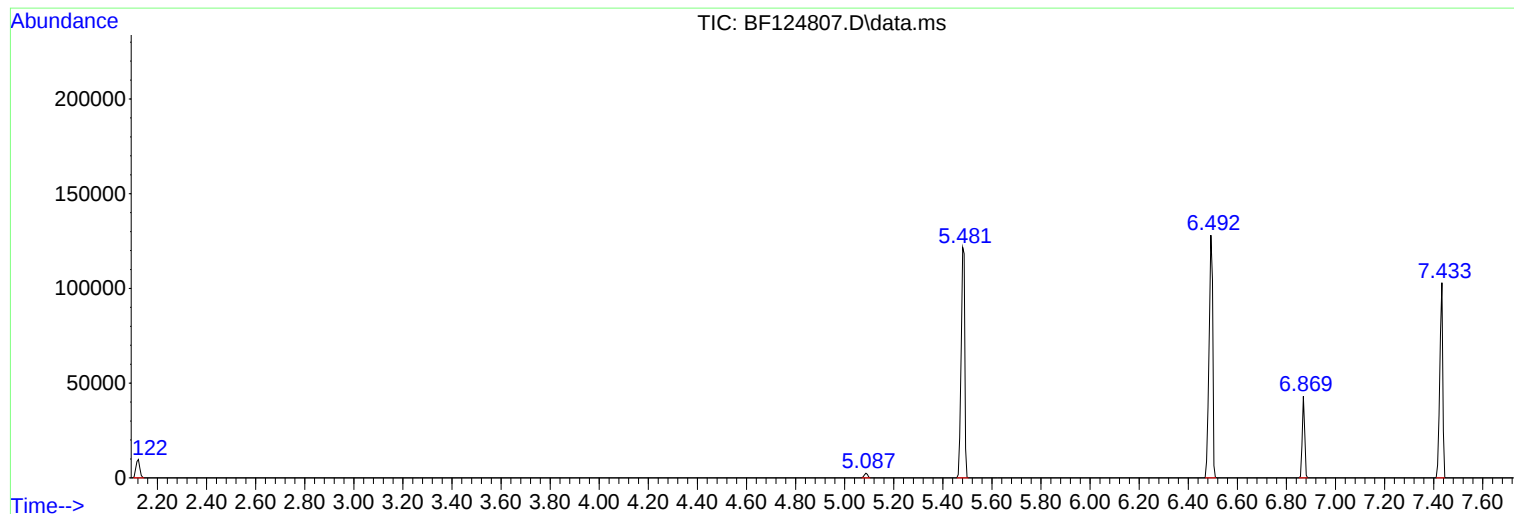
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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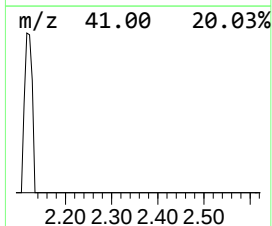
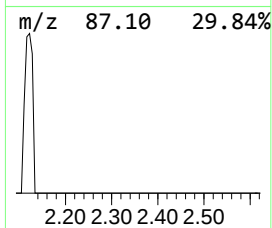
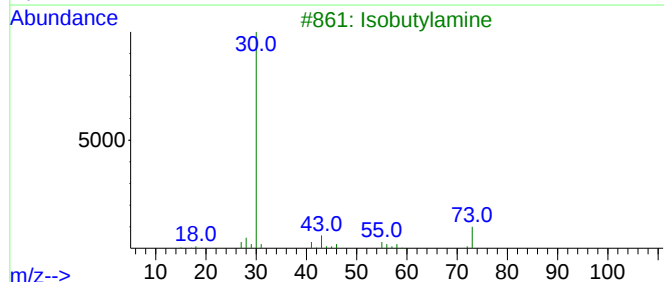
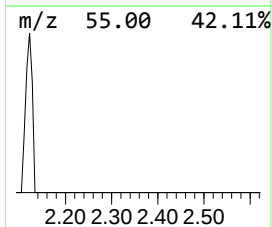
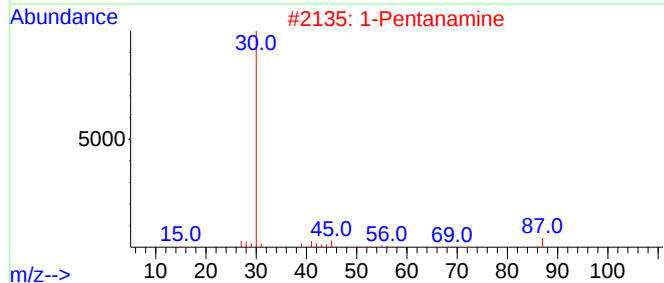
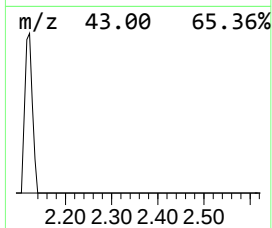
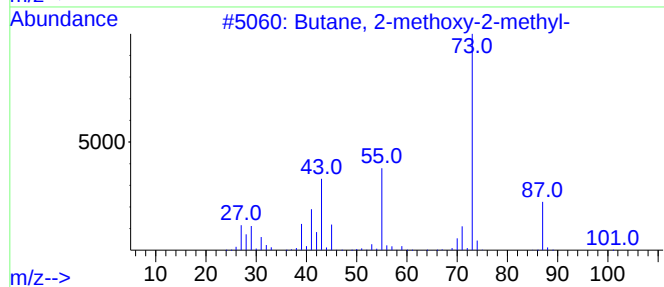
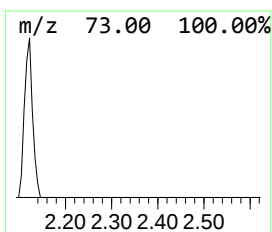
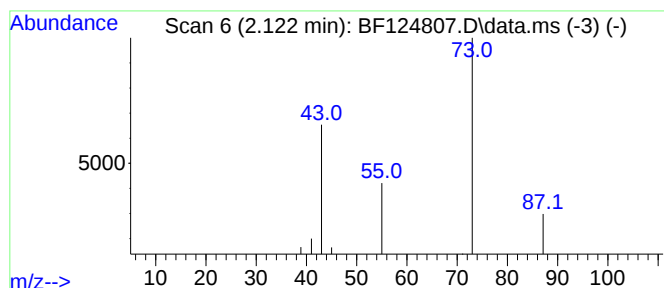
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	6.95 ng	10501	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	64
2			1-Pentanamine	87	C5H13N	000110-58-7	4
3			Isobutylamine	73	C4H11N	000078-81-9	4
4			2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	4
5			3,4-Hexanediol, 2,5-dimethyl-	146	C8H18O2	022607-11-0	4



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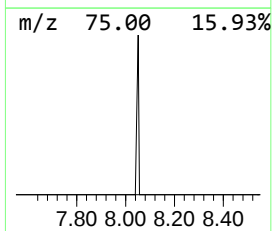
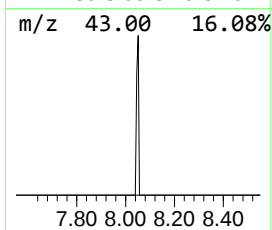
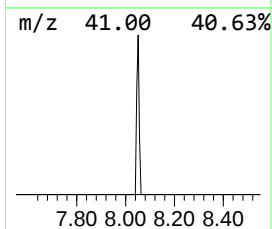
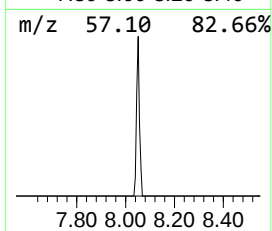
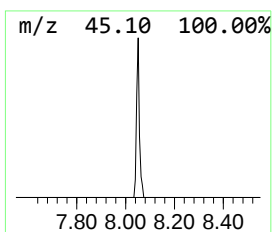
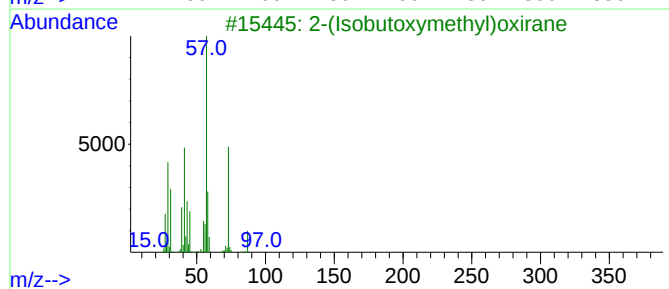
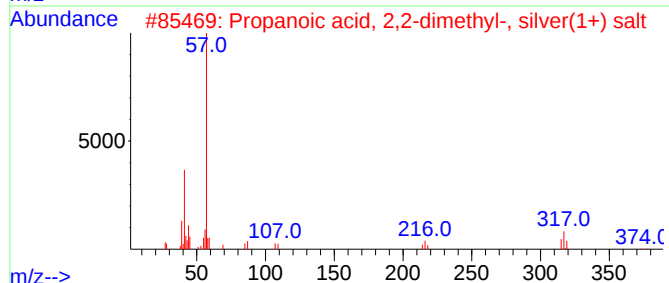
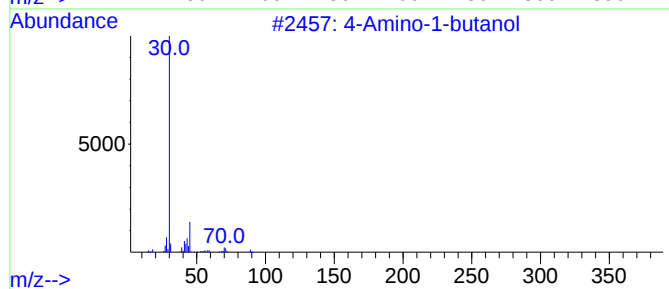
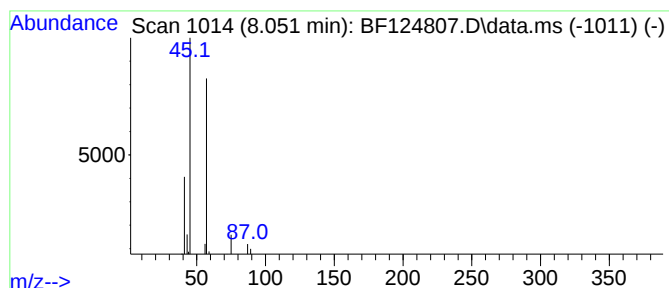
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown8.051 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	4.22 ng	9251	Naphthalene-d8	8.151

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Amino-1-butanol	89	C4H11NO	013325-10-5	9
2		Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	9
3		2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
4		di-tert-Butyl acetylenedicarboxy...	226	C12H18O4	066086-33-7	9
5		Aziridine, 1-(methoxymethyl)-	87	C4H9NO	001497-83-2	7



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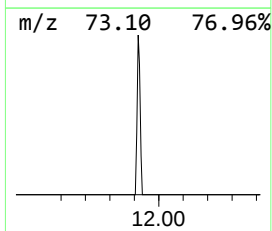
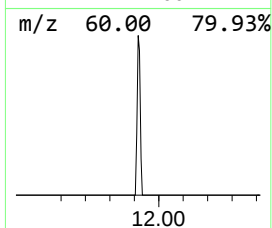
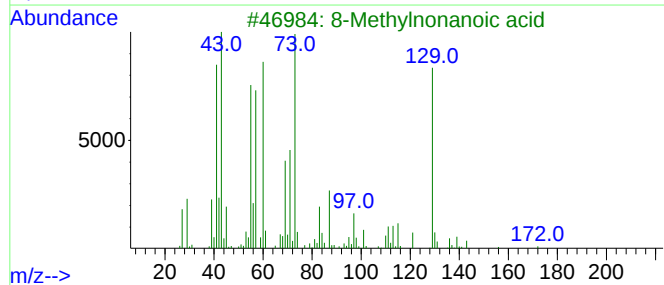
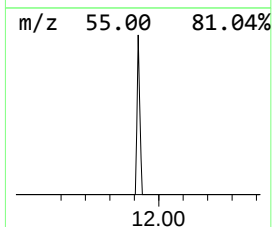
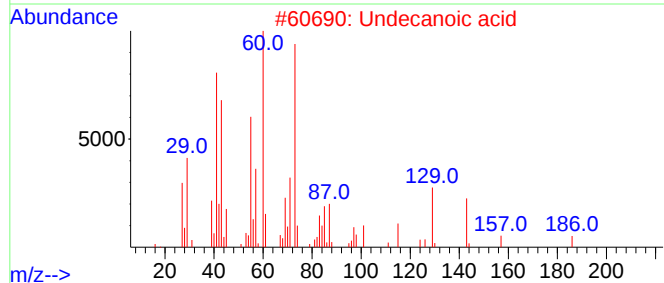
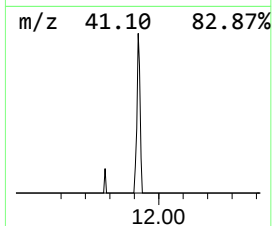
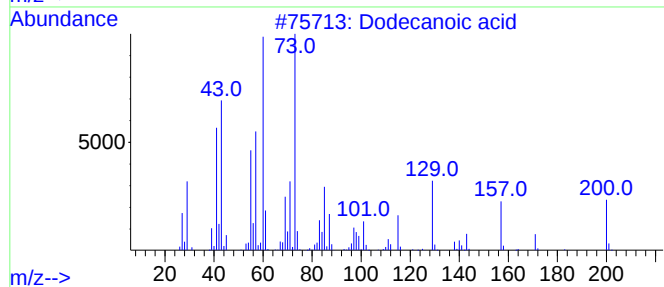
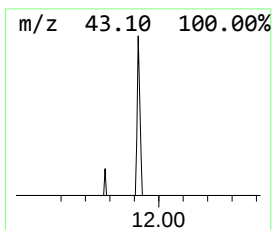
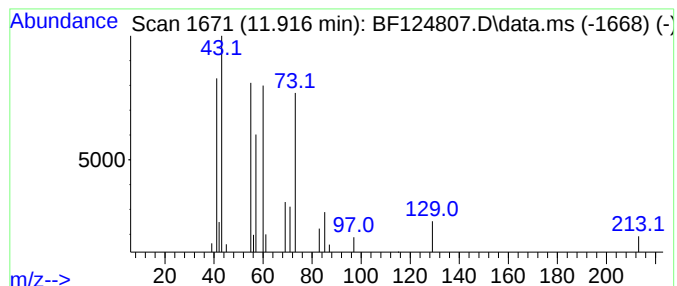
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Peak Number 3 Dodecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	5.13 ng	15274	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	64
2			Undecanoic acid	186	C11H22O2	000112-37-8	53
3			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	52
4			n-Decanoic acid	172	C10H20O2	000334-48-5	50
5			.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	43



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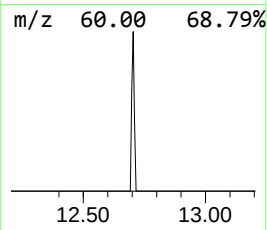
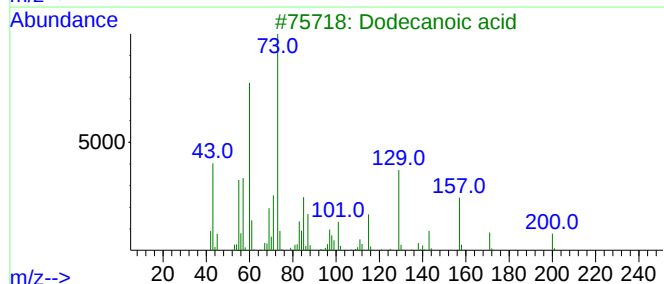
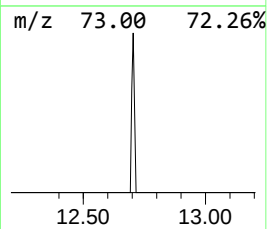
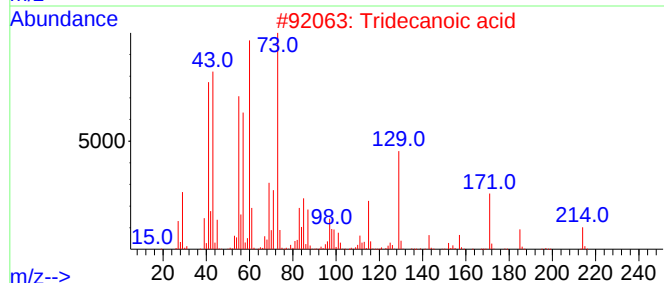
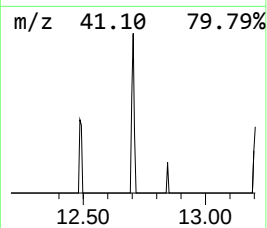
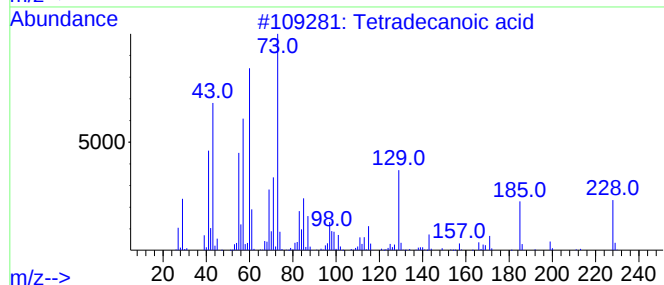
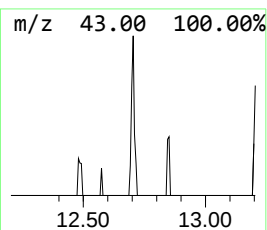
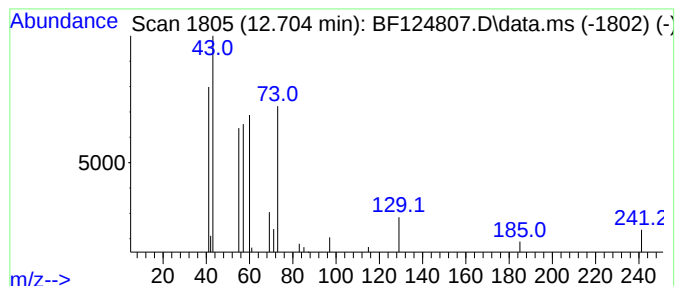
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Peak Number 4 Tetradecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	3.29 ng	9788	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
2			Tridecanoic acid	214	C13H26O2	000638-53-9	64
3			Dodecanoic acid	200	C12H24O2	000143-07-7	53
4			n-Decanoic acid	172	C10H20O2	000334-48-5	50
5			Undecanoic acid	186	C11H22O2	000112-37-8	42



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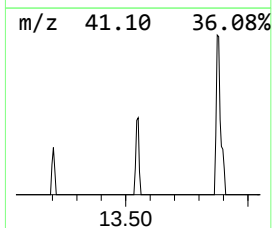
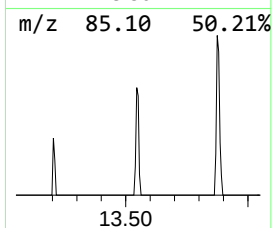
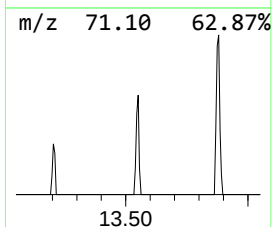
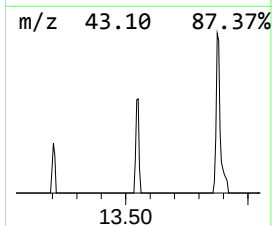
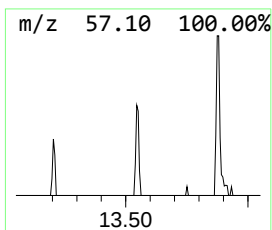
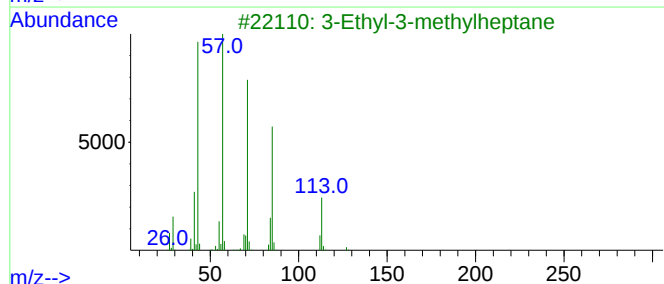
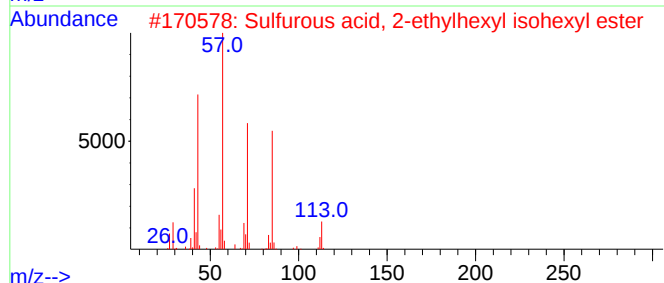
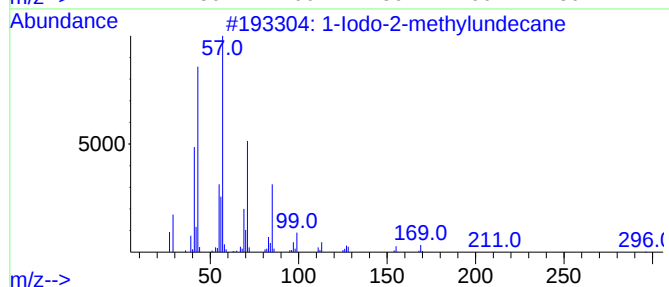
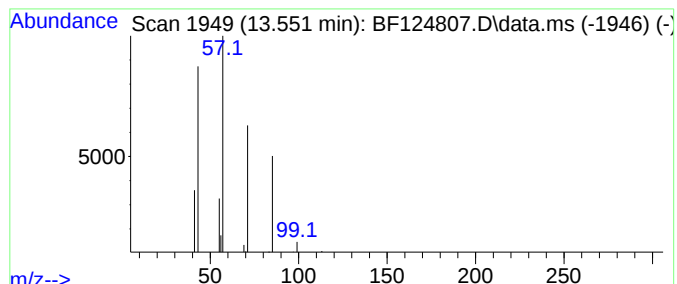
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Iodo-2-methylundecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.551	4.98 ng	12006	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	78
2			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	72
3			3-Ethyl-3-methylheptane	142	C10H22	017302-01-1	64
4			Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	64
5			Tetradecane	198	C14H30	000629-59-4	64



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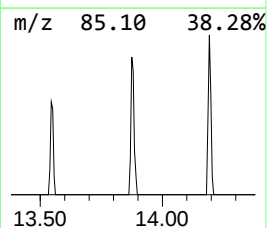
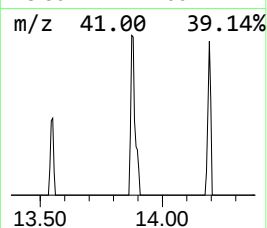
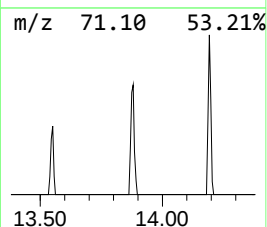
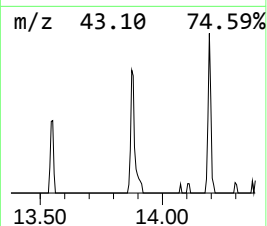
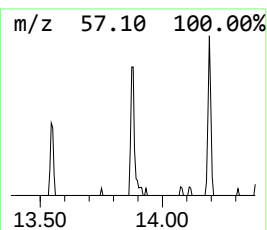
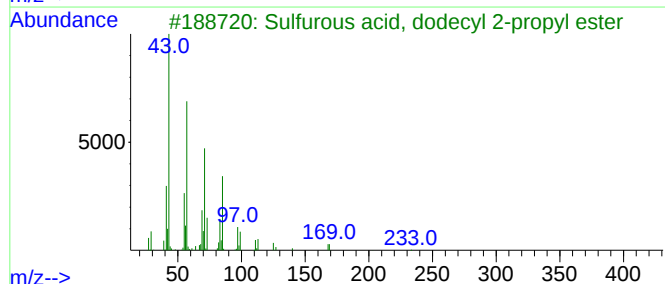
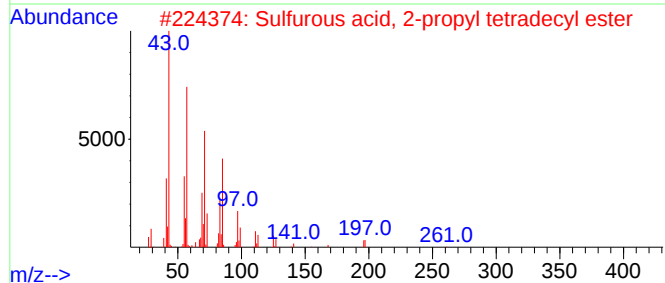
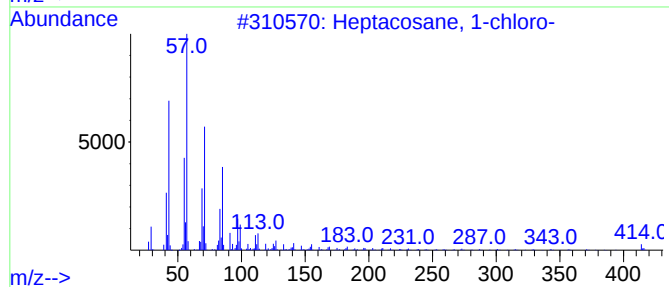
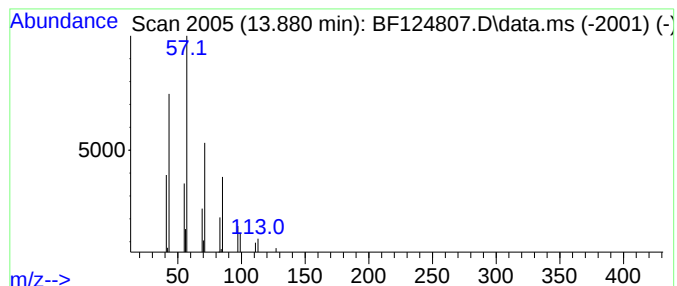
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptacosane, 1-chloro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	13.17 ng	31752	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	91
2			Sulfurous acid, 2-propyl tetradecyl ester	320	C17H36O3S	1010309-12-5	90
3			Sulfurous acid, dodecyl 2-propyl ester	292	C15H32O3S	1000309-12-3	83
4			Sulfurous acid, pentadecyl 2-propyl ester	334	C18H38O3S	1000309-12-6	78
5			Carbonic acid, octadecyl vinyl ester	340	C21H40O3	1000382-54-4	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124807.D
Acq On : 27 Jul 2021 22:40
Operator : JU/CG
Sample : M3151-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

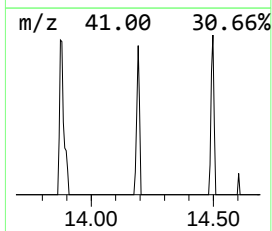
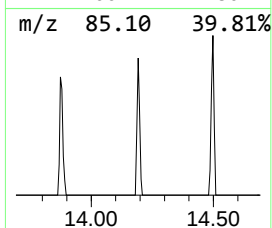
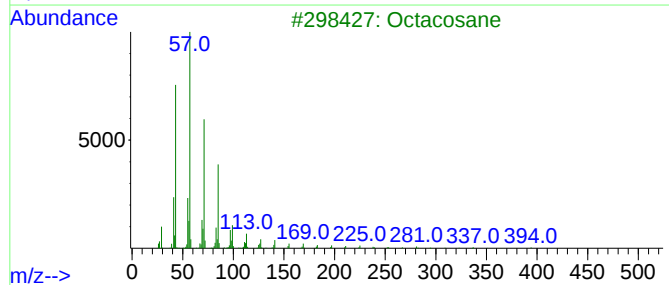
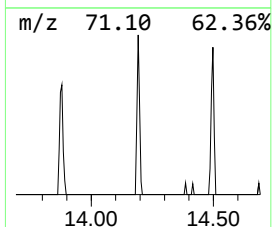
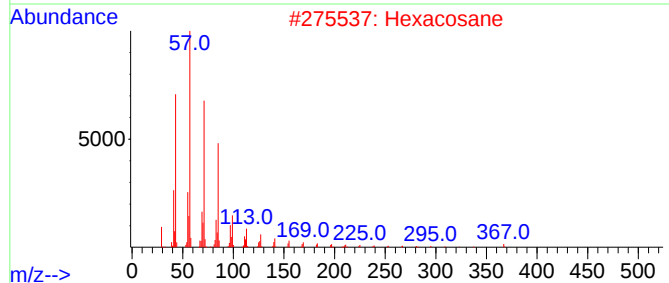
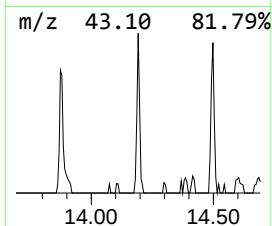
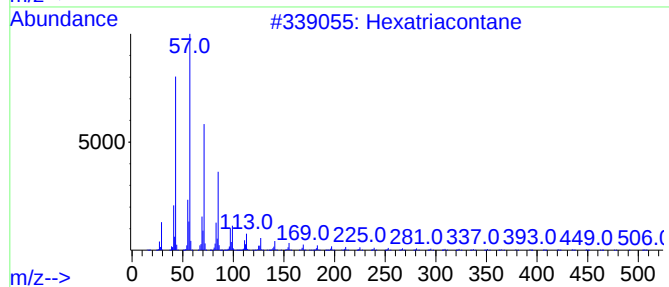
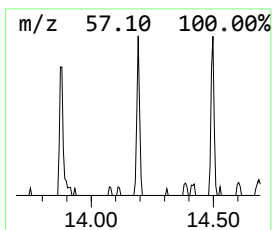
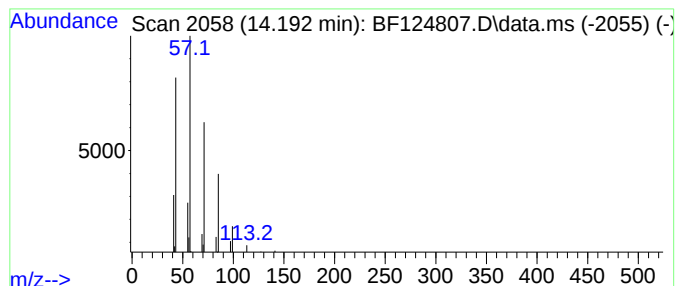
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexatriacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.192	10.35 ng	24965	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexatriacontane	507	C36H74	000630-06-8	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Octacosane	394	C28H58	000630-02-4	90
4			Tetracosane	338	C24H50	000646-31-1	90
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124807.D
Acq On : 27 Jul 2021 22:40
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Sample : M3151-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

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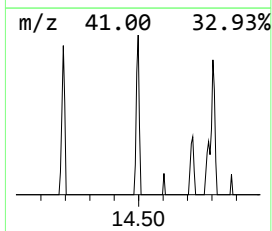
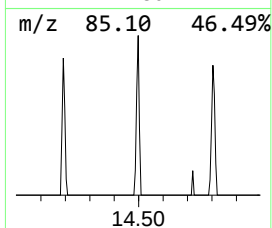
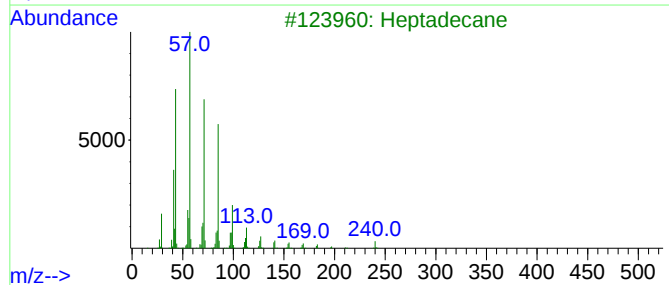
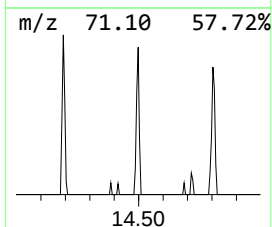
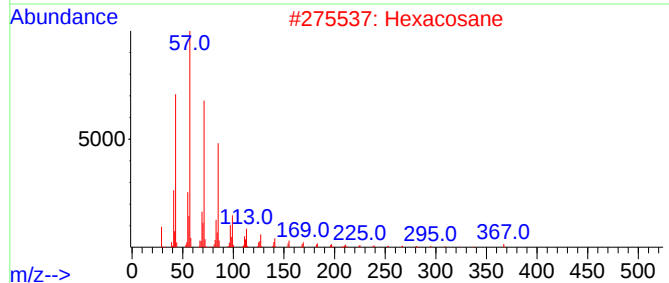
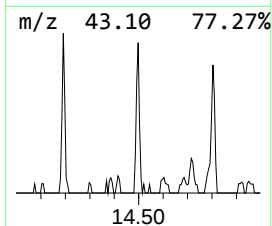
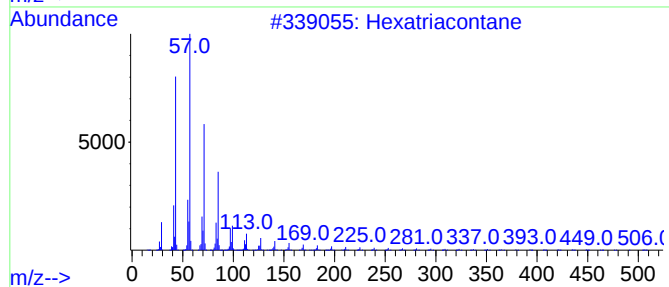
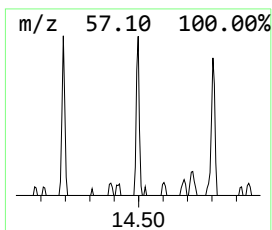
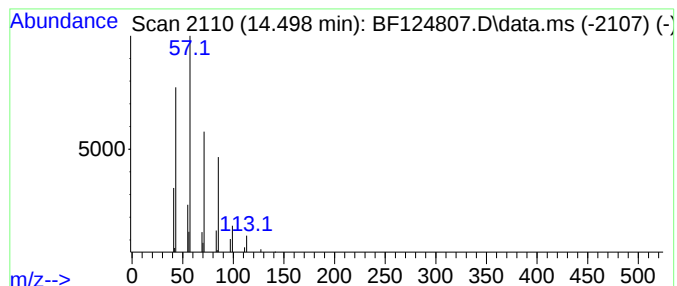
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.498	11.12 ng	26808	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexatriacontane	507	C36H74	000630-06-8	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Heptadecane	240	C17H36	000629-78-7	90
4			Tetratetracontane	619	C44H90	007098-22-8	90
5			Octacosane	394	C28H58	000630-02-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124807.D
Acq On : 27 Jul 2021 22:40
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Sample : M3151-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

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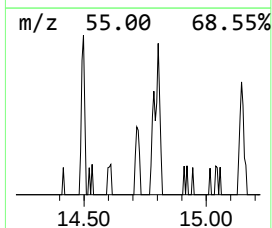
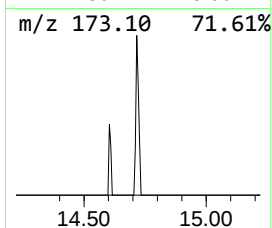
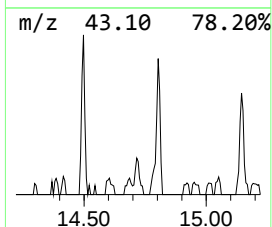
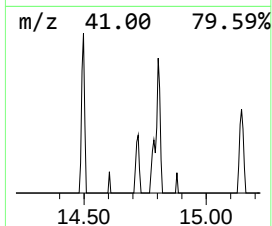
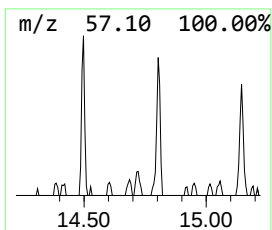
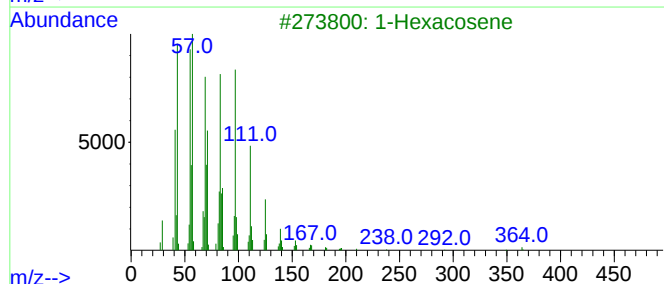
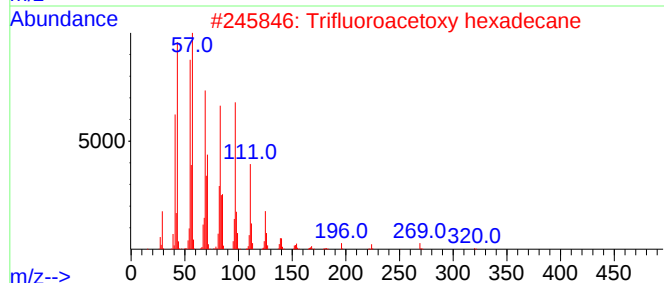
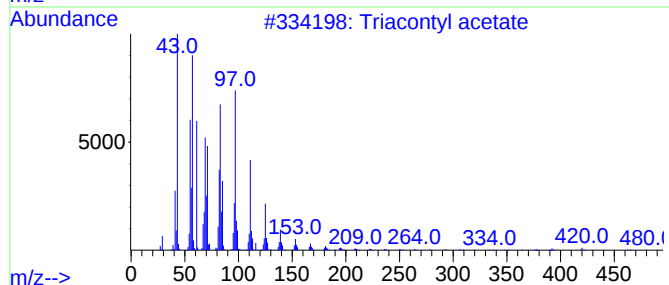
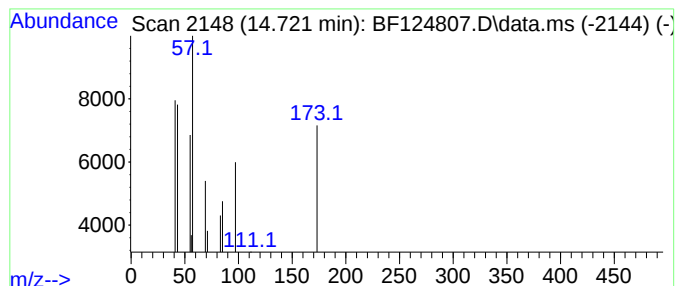
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Triacontyl acetate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.721	3.47 ng	8378	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontyl acetate	480	C32H64O2	041755-58-2	53
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	53
3			1-Hexacosene	364	C26H52	018835-33-1	53
4			Heptacosyl acetate	438	C29H58O2	1000351-78-2	50
5			Trichloroacetic acid, dodecyl ester	330	C14H25Cl3O2	074339-50-7	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124807.D
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Sample : M3151-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

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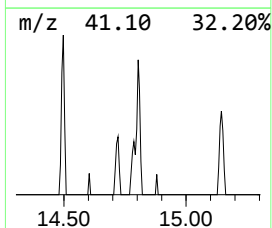
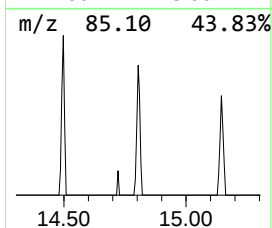
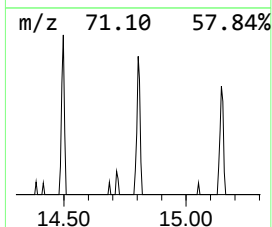
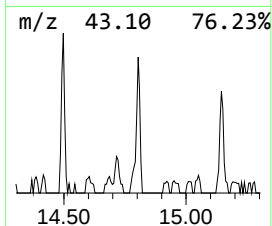
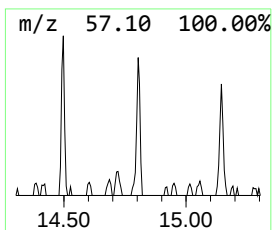
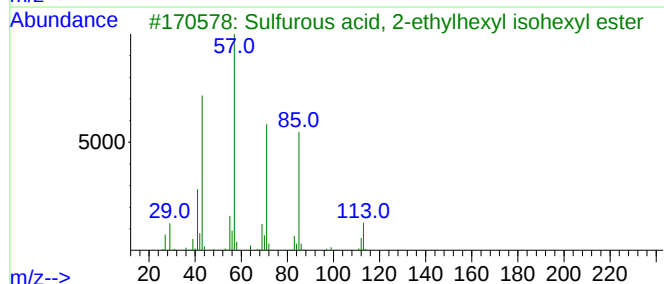
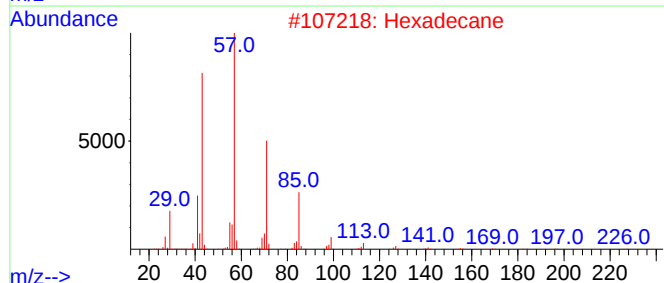
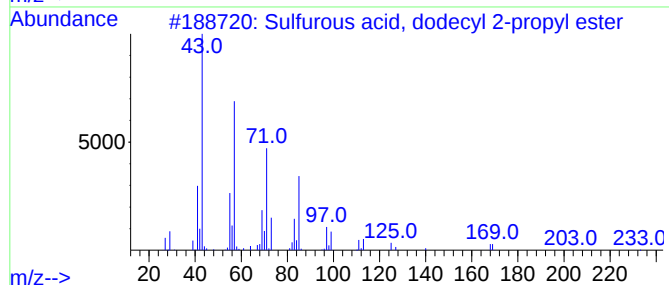
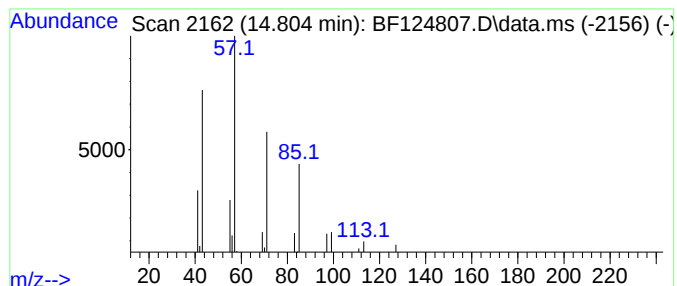
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Sulfurous acid, dodecyl 2-p... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	16.70 ng	31972	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	78
2			Hexadecane	226	C16H34	000544-76-3	72
3			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	64
4			Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	64
5			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124807.D
Acq On : 27 Jul 2021 22:40
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Sample : M3151-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

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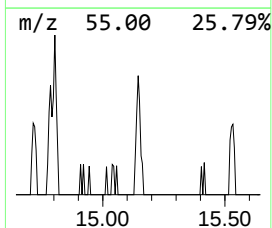
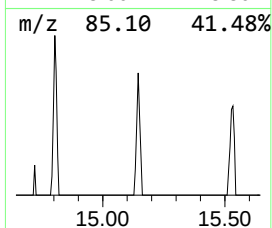
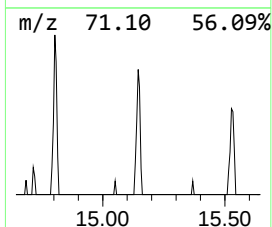
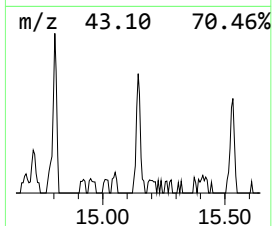
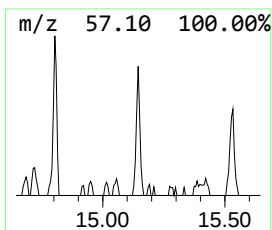
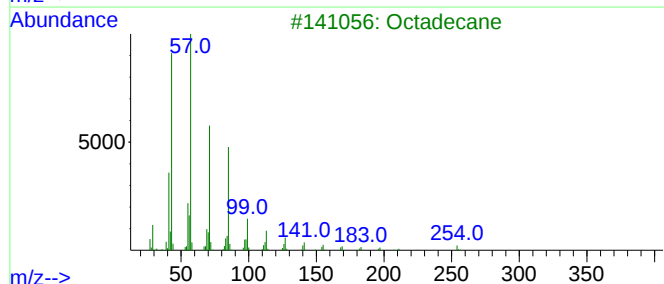
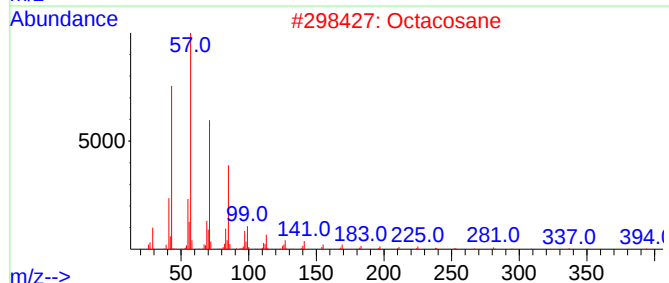
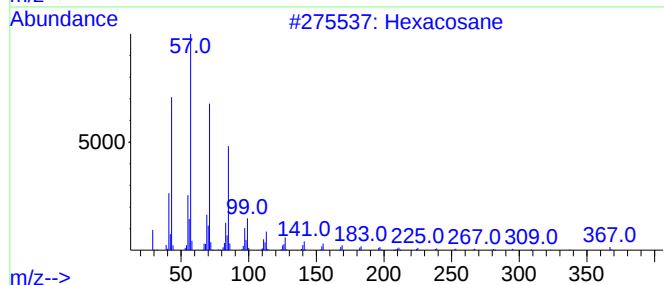
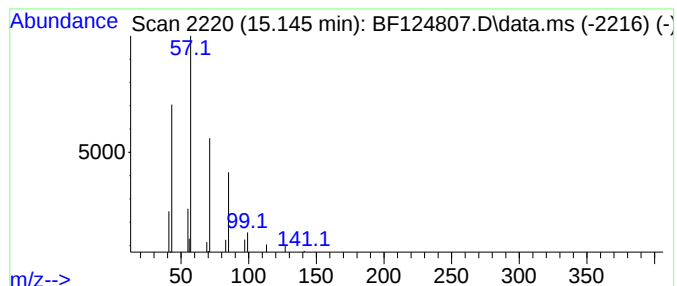
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	11.18 ng	21414	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	83
2			Octacosane	394	C28H58	000630-02-4	83
3			Octadecane	254	C18H38	000593-45-3	78
4			Heptacosane	380	C27H56	000593-49-7	78
5			Hexadecane	226	C16H34	000544-76-3	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124807.D
Acq On : 27 Jul 2021 22:40
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Misc :
ALS Vial : 12 Sample Multiplier: 1

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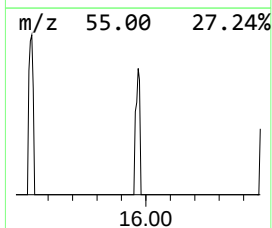
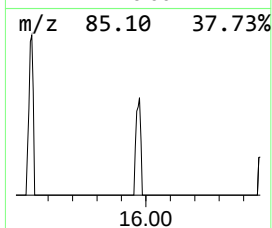
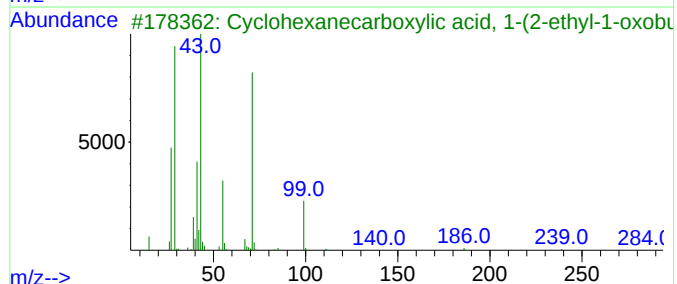
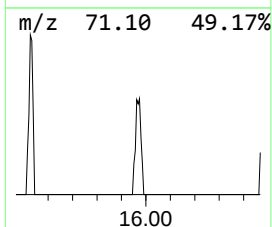
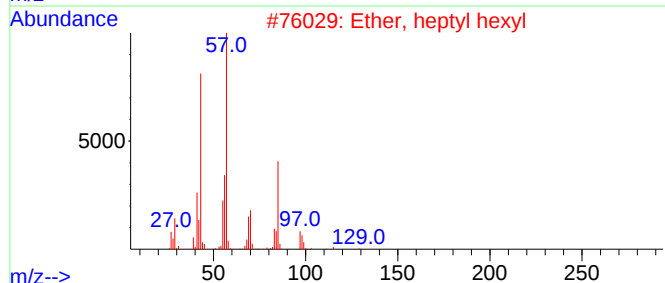
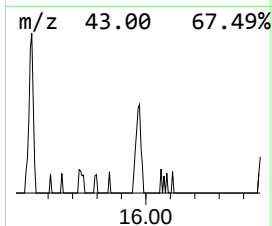
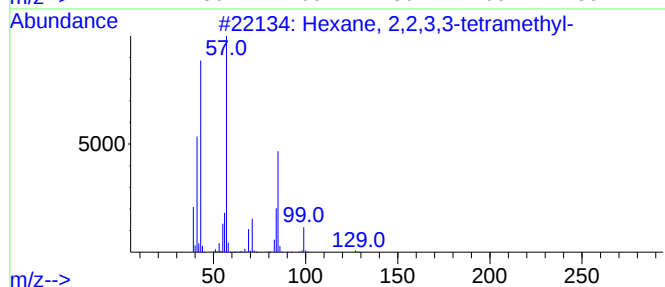
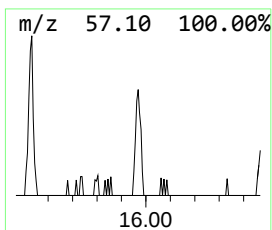
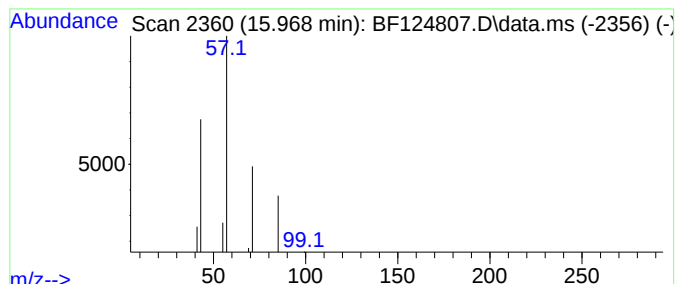
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown15.968 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.968	5.79 ng	11080	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2,3,3-tetramethyl-	142	C10H22	013475-81-5	28
2			Ether, heptyl hexyl	200	C13H28O	007289-40-9	23
3			Cyclohexanecarboxylic acid, 1-(2...	284	C15H24O5	1000460-66-2	23
4			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	9
5			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124807.D
Acq On : 27 Jul 2021 22:40
Operator : JU/CG
Sample : M3151-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

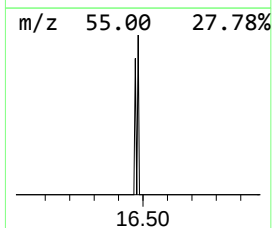
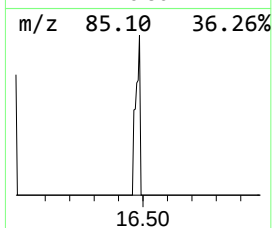
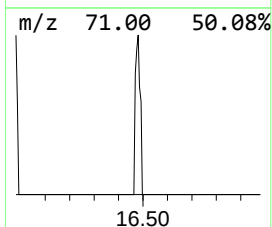
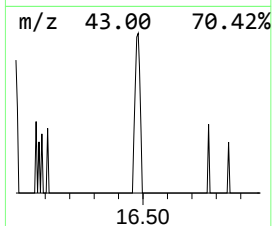
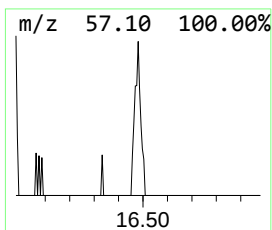
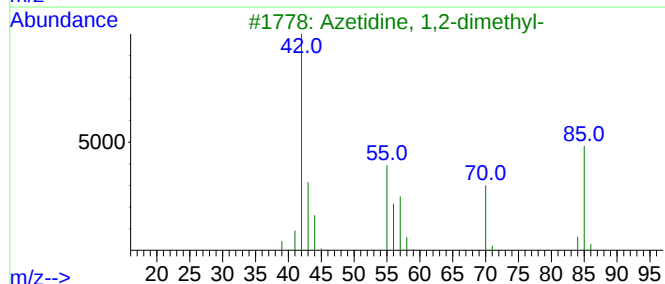
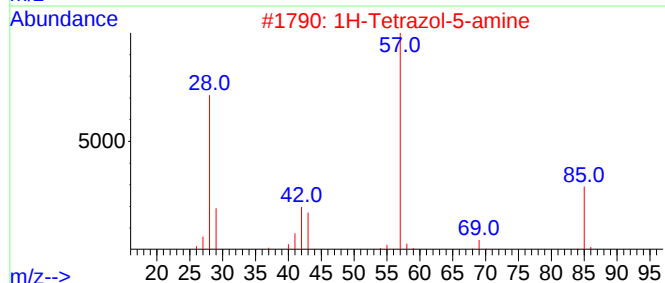
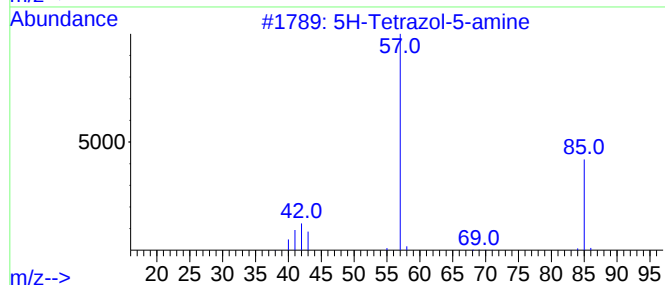
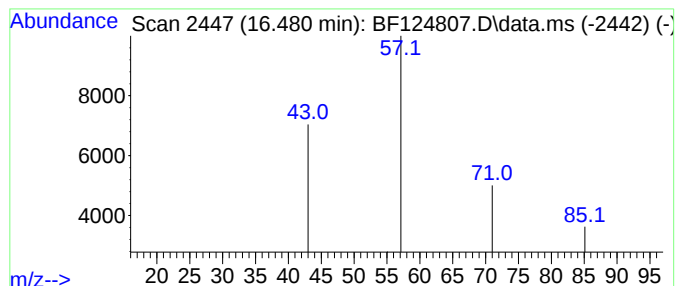
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown16.480 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.480	3.02 ng	5773	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
2			1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
3			Azetidine, 1,2-dimethyl-	85	C5H11N	051764-32-0	4
4			2-Propenamide	71	C3H5NO	000079-06-1	4
5			Oxalic acid, allyl octyl ester	242	C13H22O4	1000309-23-6	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124807.D
Acq On : 27 Jul 2021 22:40
Operator : JU/CG
Sample : M3151-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.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...	2.122	7.0	ng	10501	1	6.869	30231	20.0
unknown8.051	8.051	4.2	ng	9251	2	8.151	43846	20.0
Dodecanoic acid	11.916	5.1	ng	15274	4	11.398	59555	20.0
Tetradecanoic acid	12.704	3.3	ng	9788	4	11.398	59555	20.0
1-Iodo-2-methyl...	13.551	5.0	ng	12006	5	14.033	48228	20.0
Heptacosane, 1-...	13.880	13.2	ng	31752	5	14.033	48228	20.0
Hexatriacontane	14.192	10.4	ng	24965	5	14.033	48228	20.0
Hexacosane	14.498	11.1	ng	26808	5	14.033	48228	20.0
Triacetyl acetate	14.721	3.5	ng	8378	5	14.033	48228	20.0
Sulfurous acid,...	14.804	16.7	ng	31972	6	15.509	38291	20.0
Octacosane	15.145	11.2	ng	21414	6	15.509	38291	20.0
unknown15.968	15.968	5.8	ng	11080	6	15.509	38291	20.0
unknown16.480	16.480	3.0	ng	5773	6	15.509	38291	20.0