

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080221\
 Data File : BF124900.D
 Acq On : 2 Aug 2021 10:55
 Operator : JU/CG
 Sample : M3228-04
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20210552-COM-25

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: BF124900.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.463	571	574	580	rBB	84862	73154	83.31%	8.104%
2	6.481	743	747	750	rBV	92347	80710	91.91%	8.941%
3	6.851	808	810	813	rBB	36982	27793	31.65%	3.079%
4	7.416	902	906	909	rBB	66965	52365	59.63%	5.801%
5	8.045	1011	1013	1018	rBB	2542	2802	3.19%	0.310%
6	8.134	1025	1028	1031	rBB	48313	39581	45.07%	4.385%
7	9.210	1207	1211	1214	rBB	116758	87812	100.00%	9.728%
8	9.892	1323	1327	1329	rBB	52073	44992	51.24%	4.984%
9	10.675	1457	1460	1463	rBB	47806	33638	38.31%	3.726%
10	11.375	1576	1579	1582	rBB	63163	45955	52.33%	5.091%
11	11.892	1659	1667	1672	rBV	35419	43396	49.42%	4.807%
12	12.592	1782	1786	1787	rBV	1296	1611	1.83%	0.178%
13	12.639	1792	1794	1796	rVV	1862	1660	1.89%	0.184%
14	12.680	1796	1801	1810	rVB	33715	45904	52.28%	5.085%
15	12.822	1821	1825	1828	rBV	738	1481	1.69%	0.164%
16	12.957	1844	1848	1851	rBV	114499	87526	99.67%	9.696%
17	13.327	1899	1911	1919	rBB3	17270	51564	58.72%	5.712%
18	13.480	1934	1937	1940	rBB	807	1138	1.30%	0.126%
19	13.904	2003	2009	2011	rBV	2128	2829	3.22%	0.313%
20	14.010	2024	2027	2031	rBB	42761	34233	38.98%	3.792%
21	14.216	2056	2062	2069	rBB2	20462	36838	41.95%	4.081%
22	14.474	2103	2106	2109	rBB	1769	1667	1.90%	0.185%
23	14.780	2155	2158	2160	rBB	3105	2786	3.17%	0.309%
24	14.892	2170	2177	2183	rBB2	10386	20389	23.22%	2.259%
25	15.115	2212	2215	2218	rVB	4612	5564	6.34%	0.616%
26	15.351	2251	2255	2256	rBV2	2732	3237	3.69%	0.359%
27	15.480	2272	2277	2283	rVB2	20575	28201	32.12%	3.124%
28	15.645	2296	2305	2310	rBB3	4806	12842	14.62%	1.423%
29	15.927	2349	2353	2357	rBB2	3689	5832	6.64%	0.646%
30	16.439	2435	2440	2442	rBB2	2677	3010	3.43%	0.333%
31	16.515	2445	2453	2459	rBB2	4098	10146	11.55%	1.124%
32	17.533	2623	2626	2634	rVB4	3213	7021	8.00%	0.778%
33	18.745	2828	2832	2833	rBV2	1105	1517	1.73%	0.168%
34	18.756	2833	2834	2842	rVB2	1913	3508	3.99%	0.389%

Sum of corrected areas: 902702

Instrument :

BNA_F

ClientSampleId :

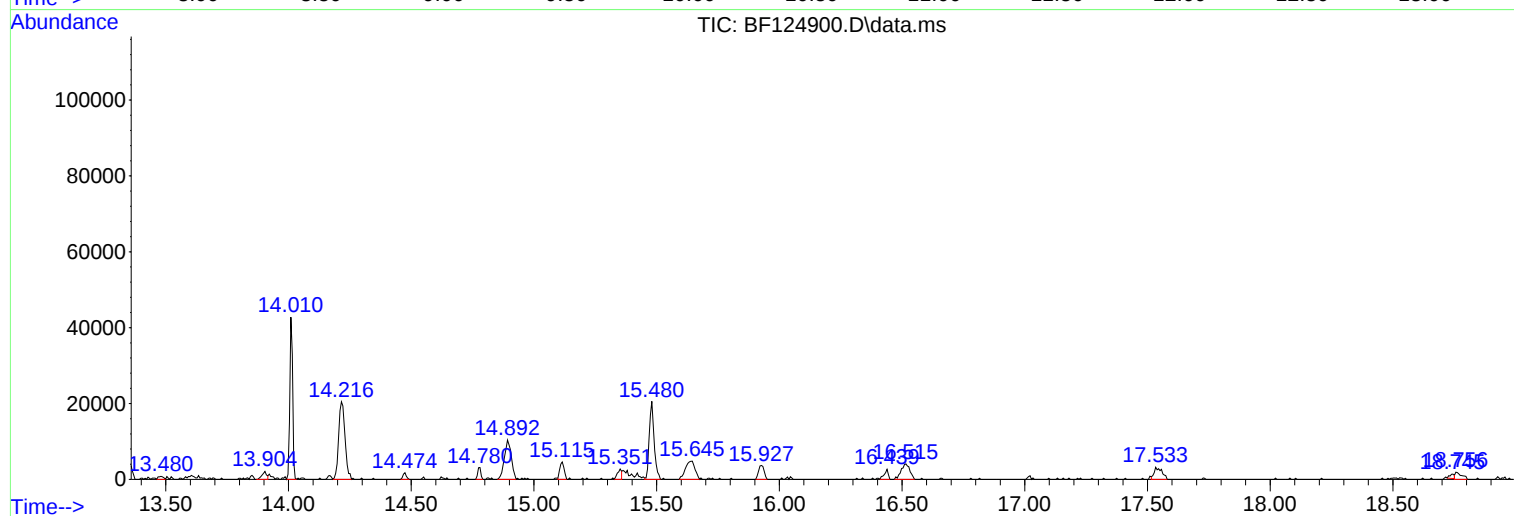
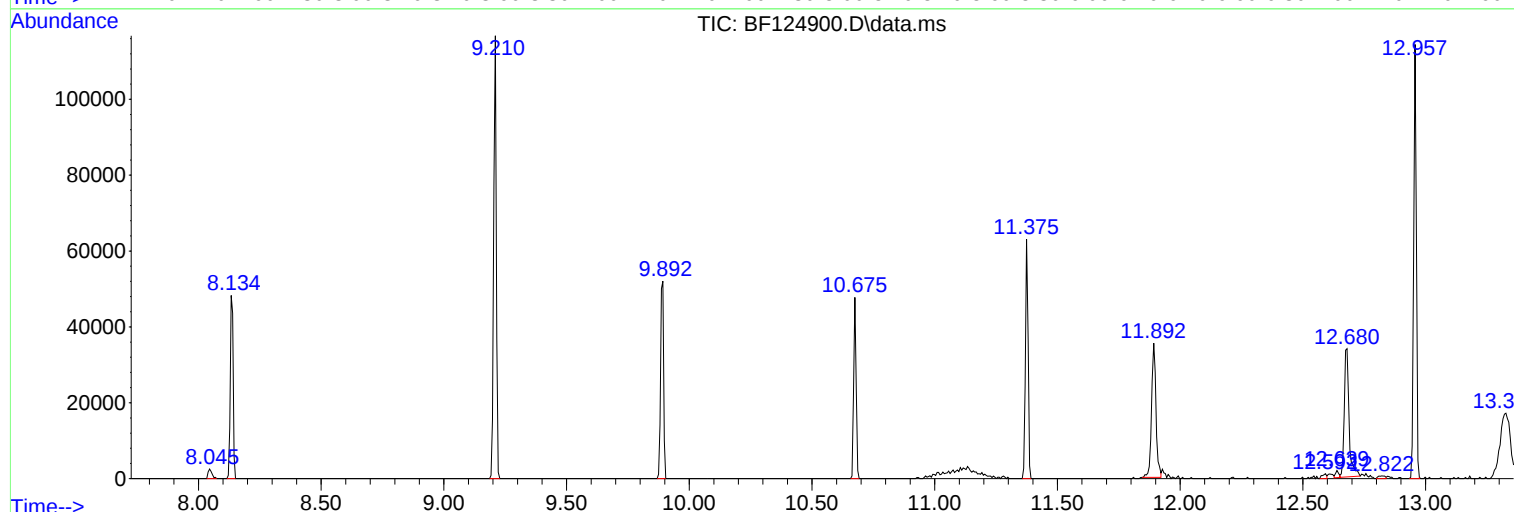
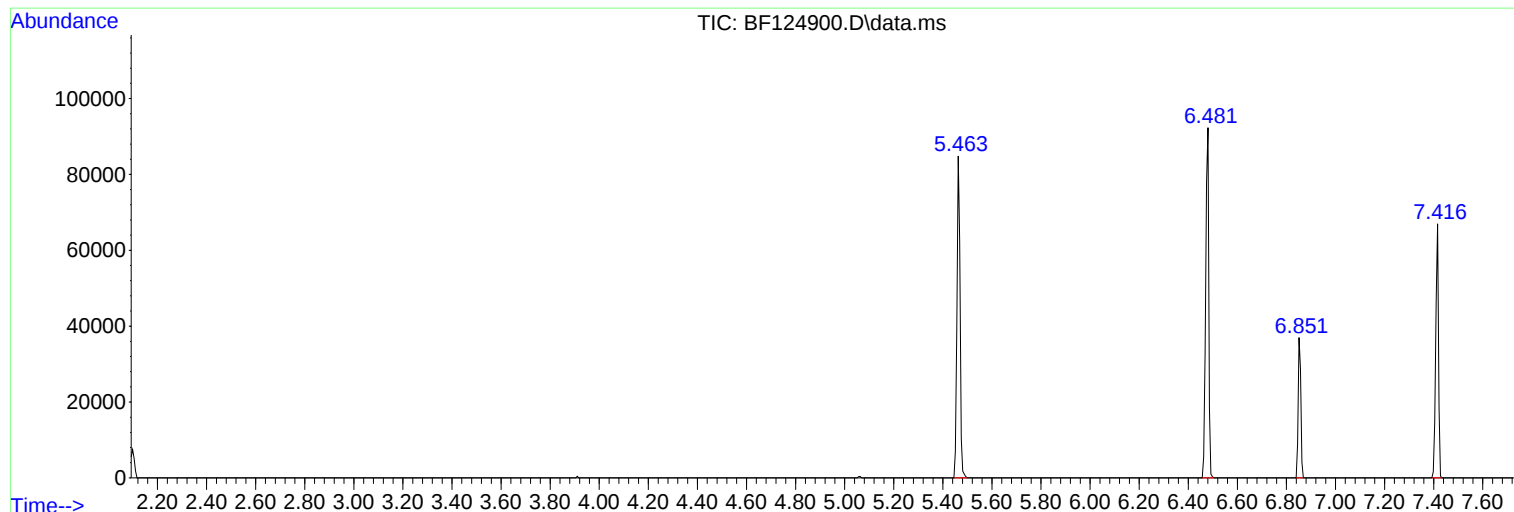
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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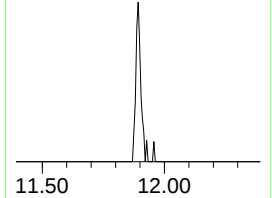
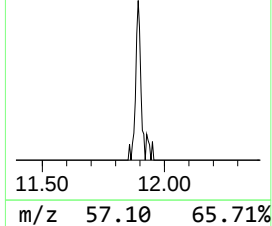
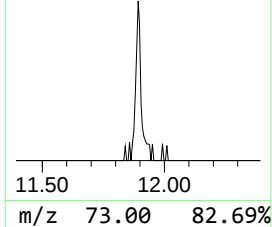
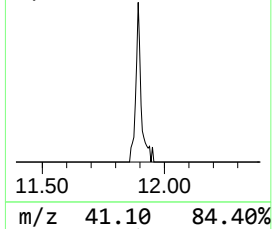
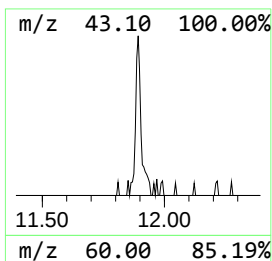
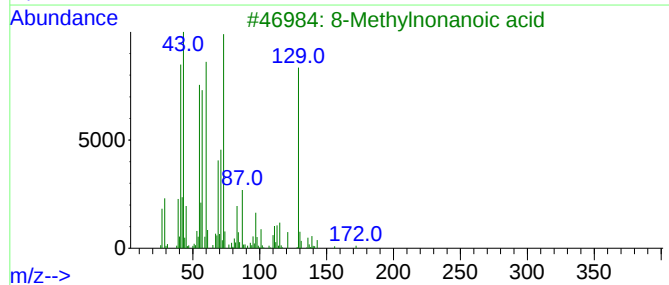
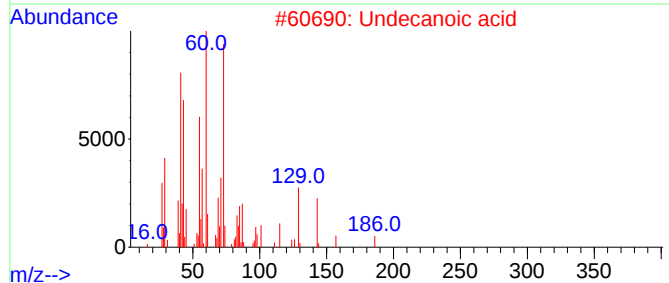
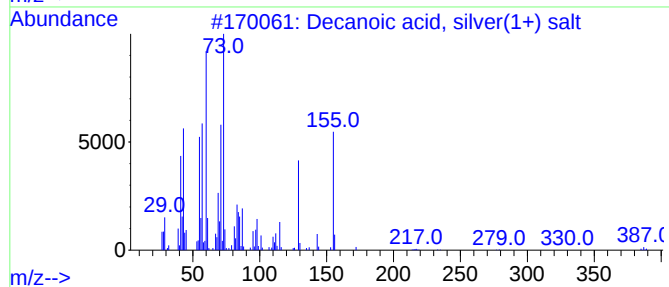
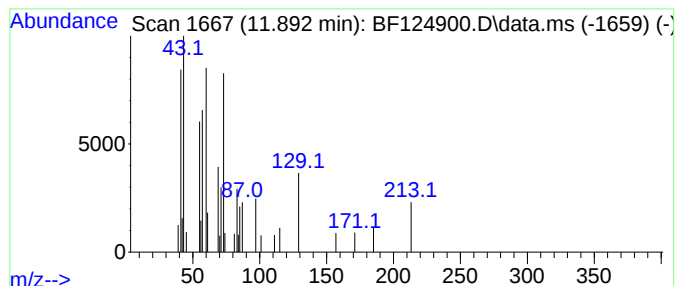
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Decanoic acid, silver(1+) salt Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.892	18.89 ng	43396	Phenanthrene-d10		11.374	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Decanoic acid, silver(1+) salt		278	C10H19AgO2	013126-67-5	53
2	Undecanoic acid		186	C11H22O2	000112-37-8	50
3	8-Methylnonanoic acid		172	C10H20O2	005963-14-4	50
4	n-Decanoic acid		172	C10H20O2	000334-48-5	43
5	Octanoic acid, silver(1+) salt		250	C8H15AgO2	024927-67-1	37



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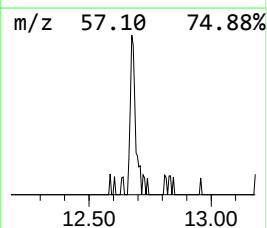
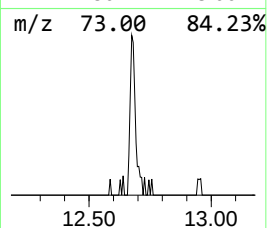
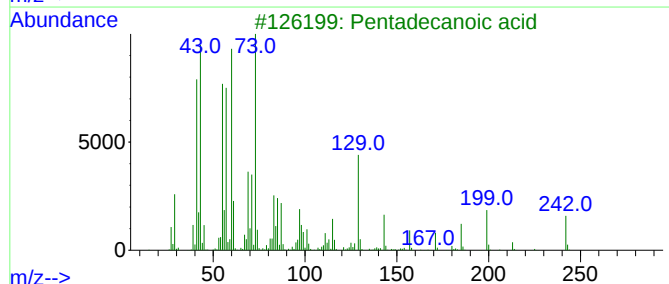
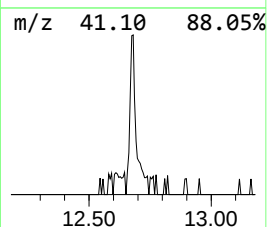
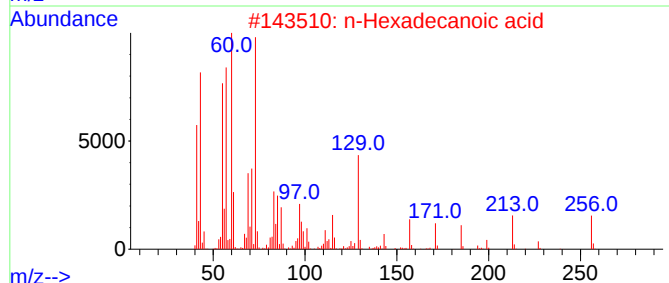
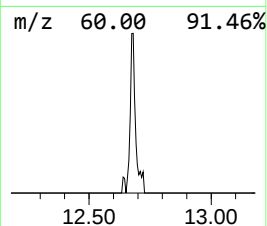
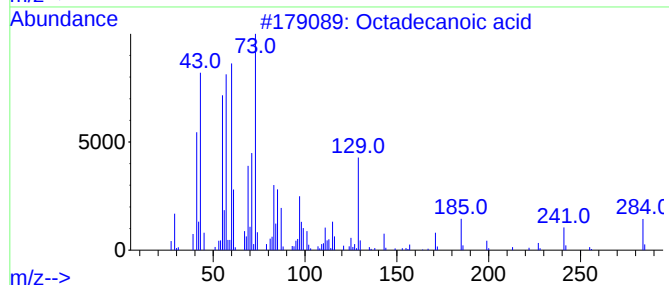
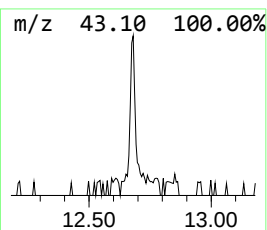
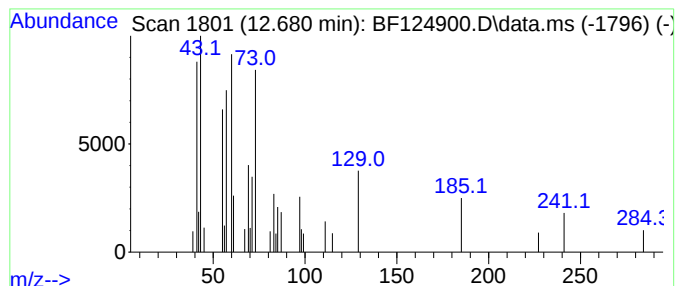
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.680	19.98 ng	45904	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Tridecanoic acid	214	C13H26O2	000638-53-9	58



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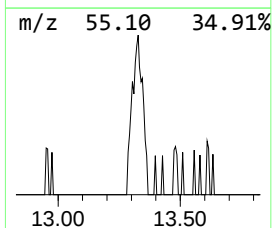
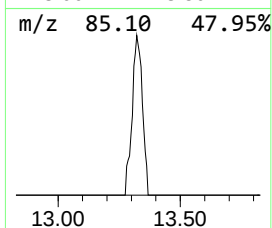
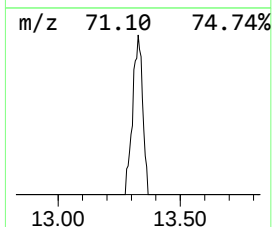
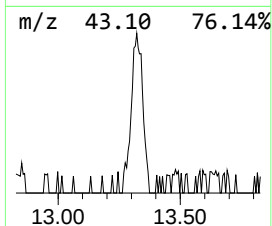
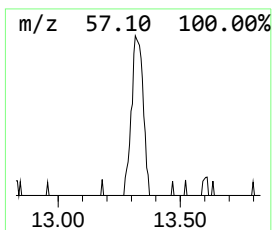
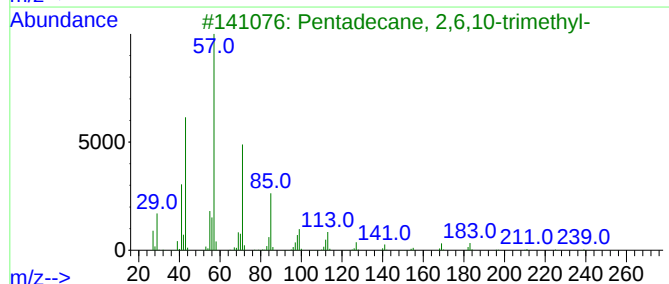
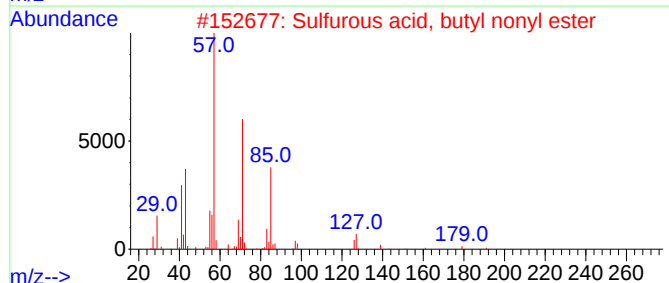
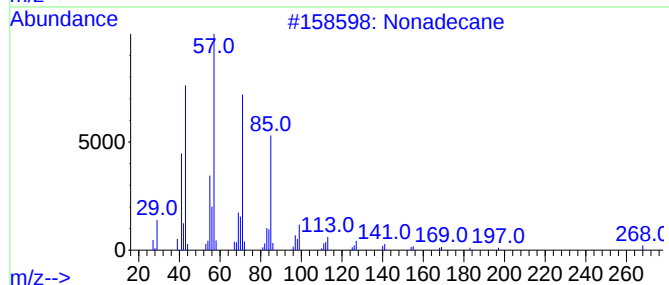
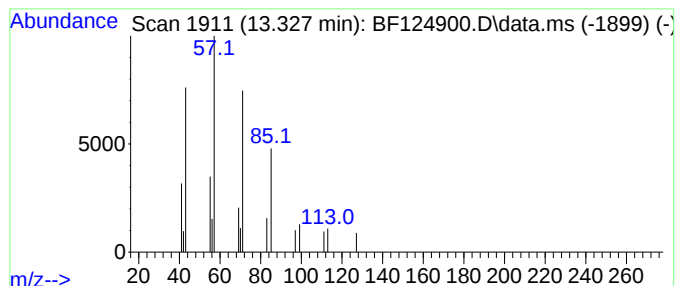
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Peak Number 3 Nonadecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.327	30.13 ng	51564	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	78
2			Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	72
3			Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	72
4			Tridecane	184	C13H28	000629-50-5	72
5			Tetradecane	198	C14H30	000629-59-4	64



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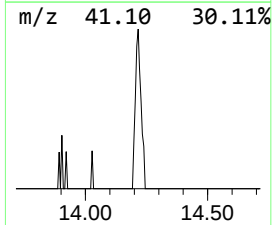
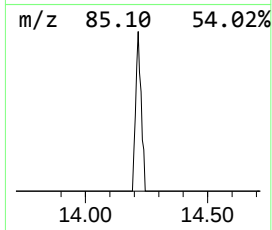
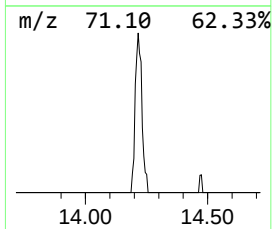
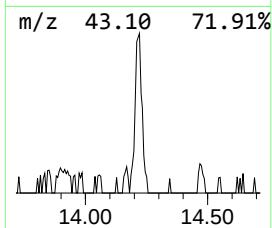
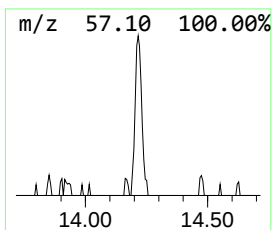
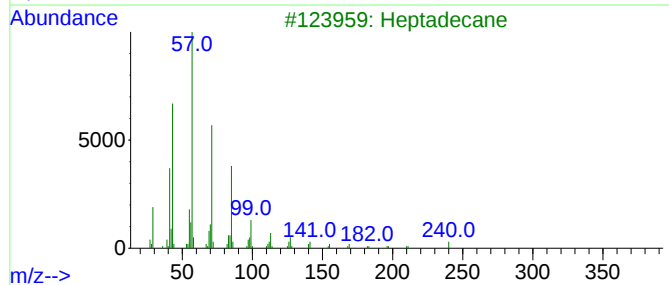
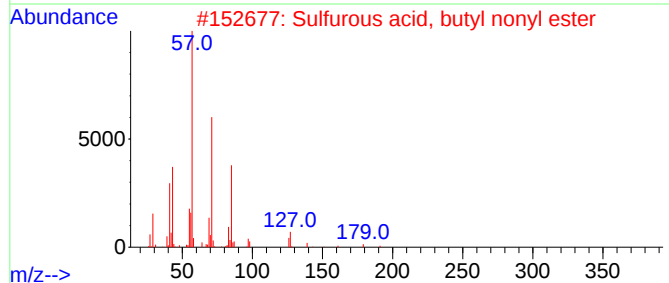
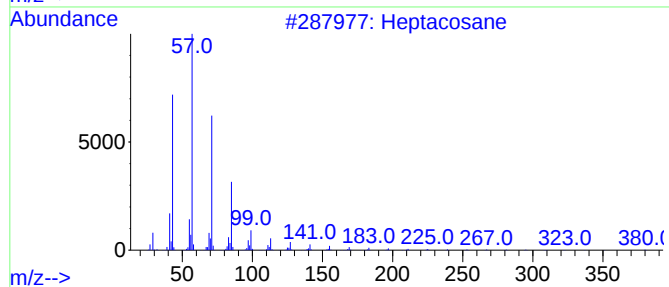
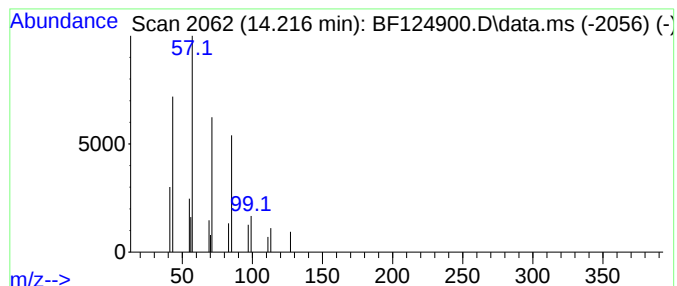
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Peak Number 4 Heptacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.216	21.52 ng	36838	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	83
2			Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	64
3			Heptadecane	240	C17H36	000629-78-7	64
4			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	59
5			Octane, 3,4,5,6-tetramethyl-	170	C12H26	062185-21-1	59



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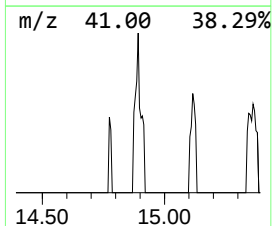
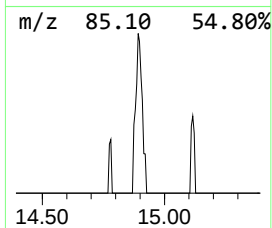
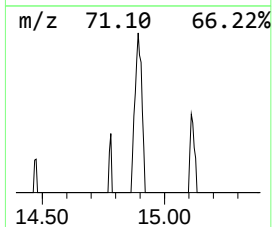
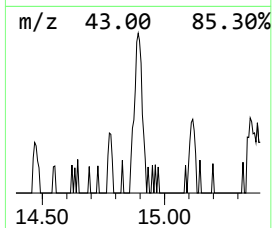
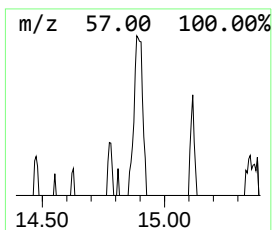
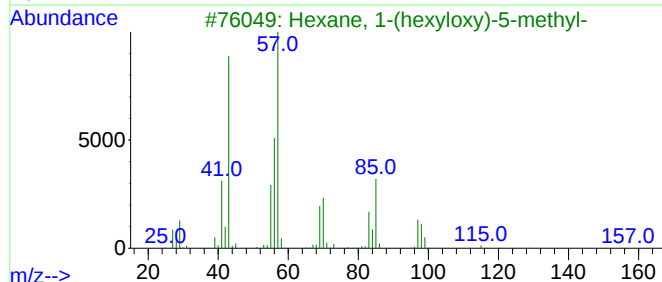
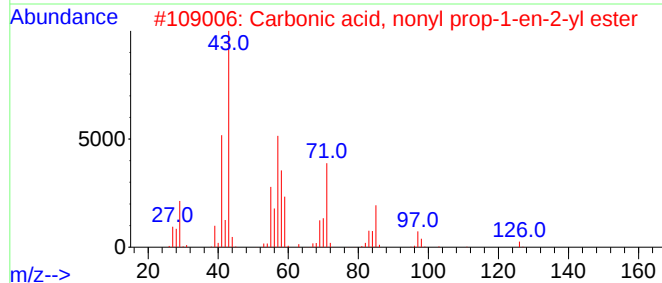
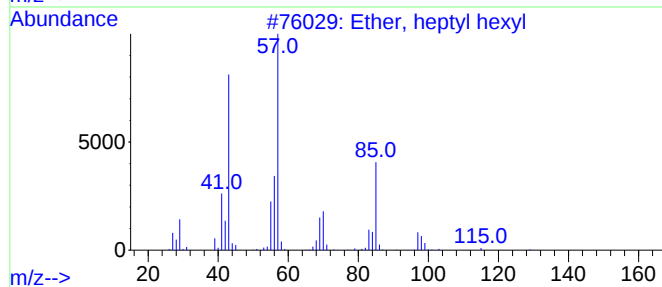
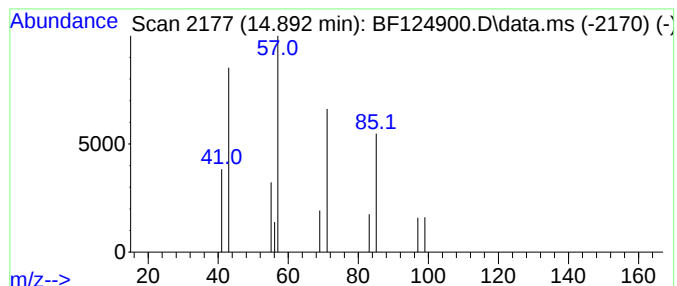
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Peak Number 5 unknown14.892 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.892	14.46 ng	20389	Perylene-d12	15.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ether, heptyl hexyl	200	C13H28O	007289-40-9	38
2			Carbonic acid, nonyl prop-1-en-2...	228	C13H24O3	1000382-53-9	36
3			Hexane, 1-(hexyloxy)-5-methyl-	200	C13H28O	074421-19-5	25
4			2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	12
5			Heptane, 2,2,3,3,5,6,6-heptamethyl-	198	C14H30	007225-67-4	12



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ClientSampleId :
20210552-COM-25

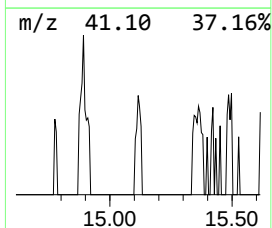
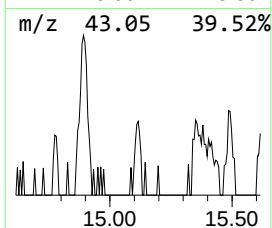
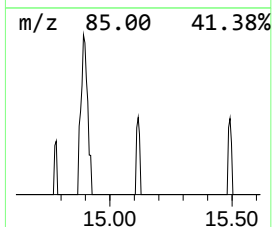
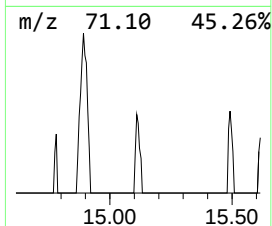
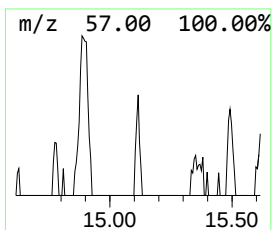
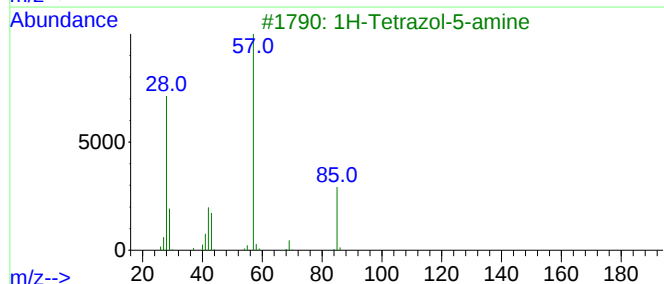
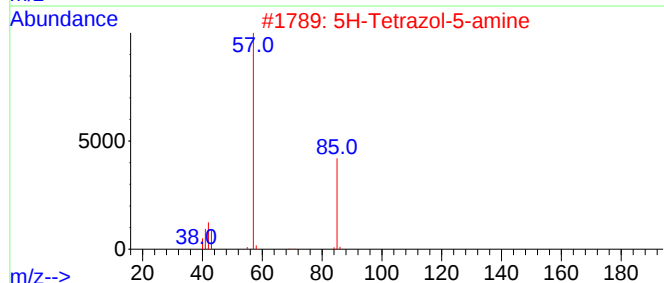
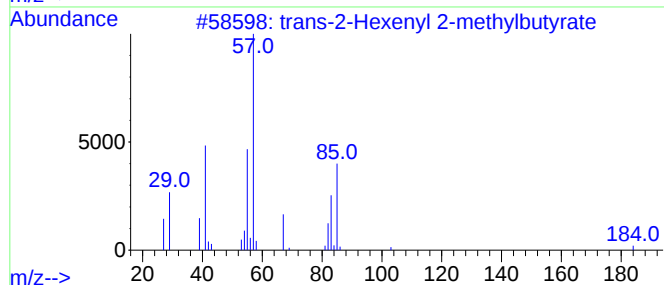
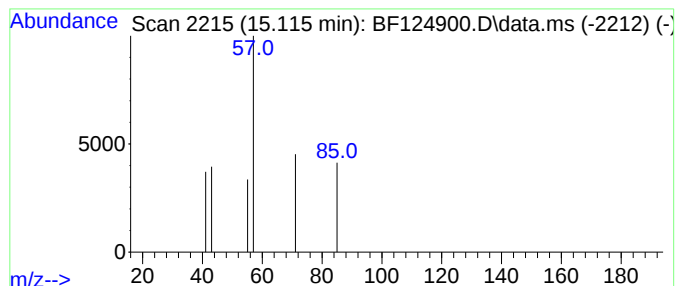
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown15.116 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.116	3.95 ng	5564	Perylene-d12	15.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-2-Hexenyl 2-methylbutyrate	184	C11H20O2	1000433-23-8	9
2			5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
3			1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
4			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	3
5			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080221\
Data File : BF124900.D
Acq On : 2 Aug 2021 10:55
Operator : JU/CG
Sample : M3228-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

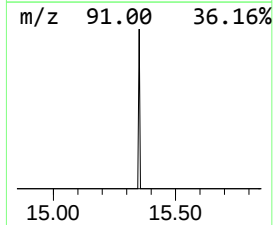
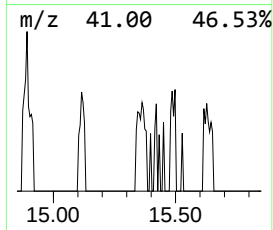
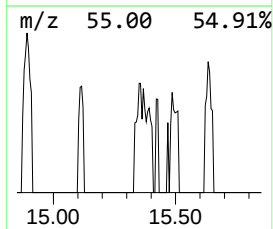
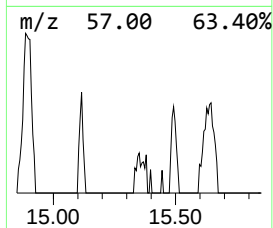
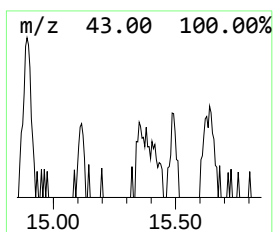
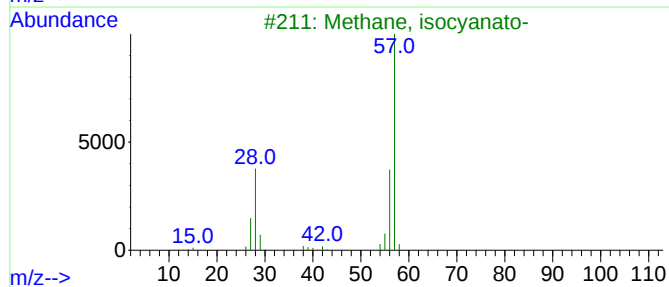
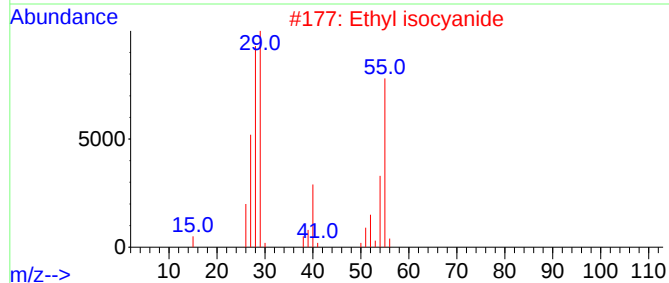
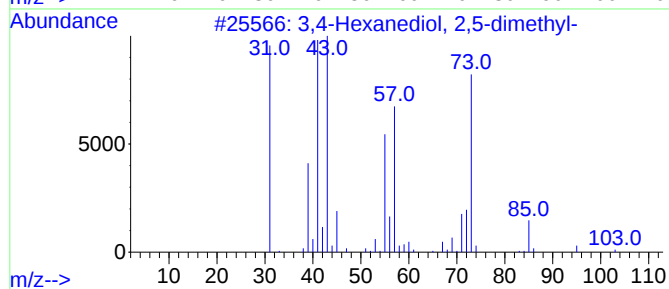
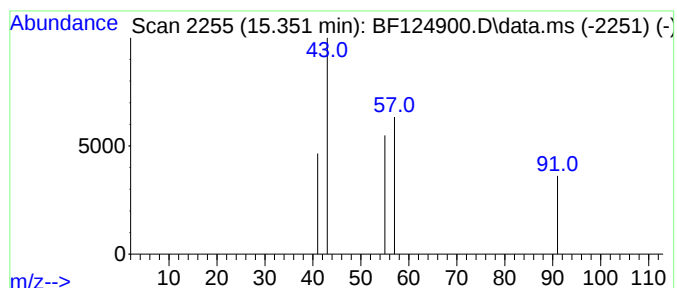
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ClientSampleId :
20210552-COM-25

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 7 unknown15.351 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.351	2.30 ng	3237	Perylene-d12	15.480	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Hexanediol, 2,5-dimethyl-	146	C8H18O2	022607-11-0	2
2	Ethyl isocyanide	55	C3H5N	000624-79-3	1
3	Methane, isocyanato-	57	C2H3NO	000624-83-9	1
4	Azetidine	57	C3H7N	000503-29-7	1
5	Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	1



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080221\
Data File : BF124900.D
Acq On : 2 Aug 2021 10:55
Operator : JU/CG
Sample : M3228-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210552-COM-25

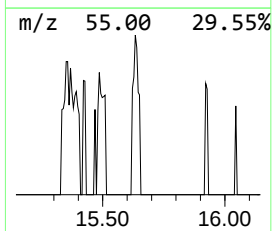
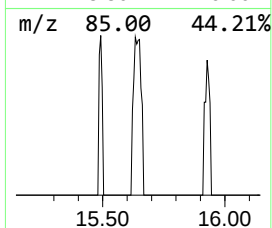
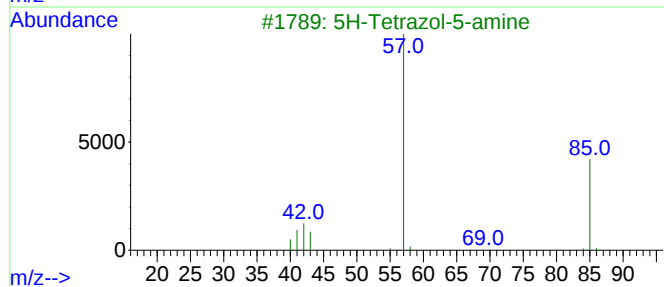
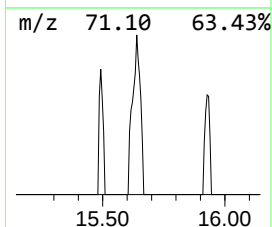
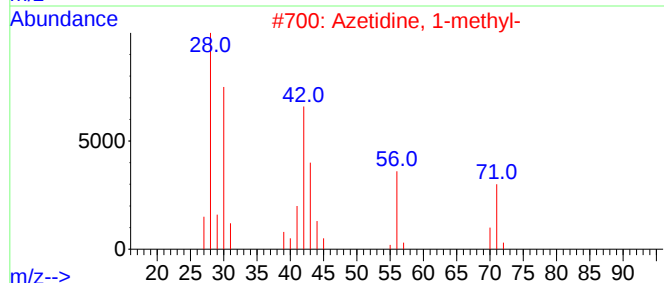
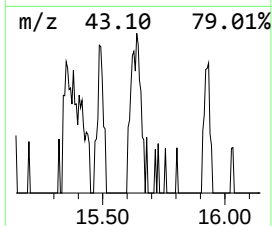
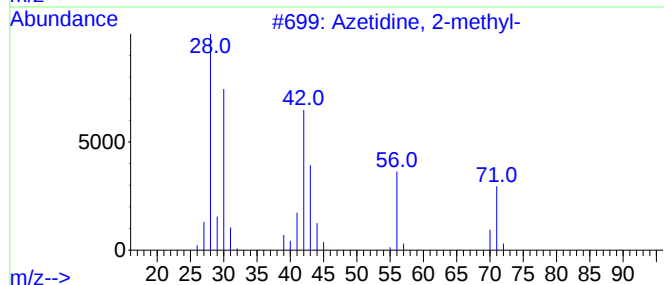
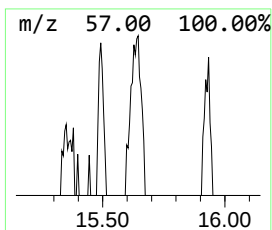
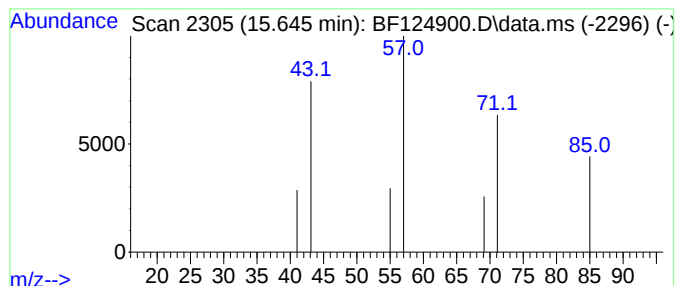
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.645 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.645	9.11 ng	12842	Perylene-d12	15.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
2			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
3			5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
4			2-Propenamide	71	C3H5NO	000079-06-1	4
5			Oxalic acid, isohexyl neopentyl ...	244	C13H24O4	1000309-73-0	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080221\
Data File : BF124900.D
Acq On : 2 Aug 2021 10:55
Operator : JU/CG
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Misc :
ALS Vial : 4 Sample Multiplier: 1

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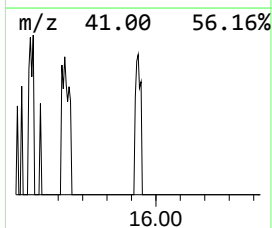
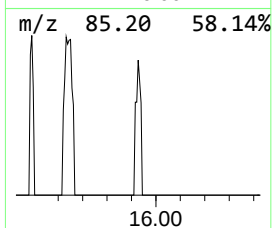
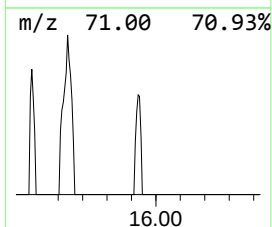
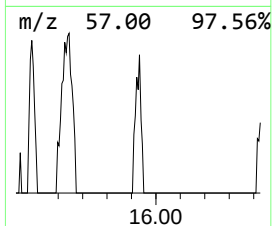
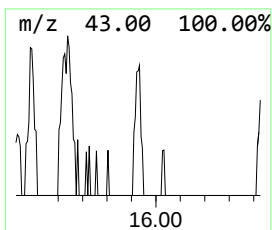
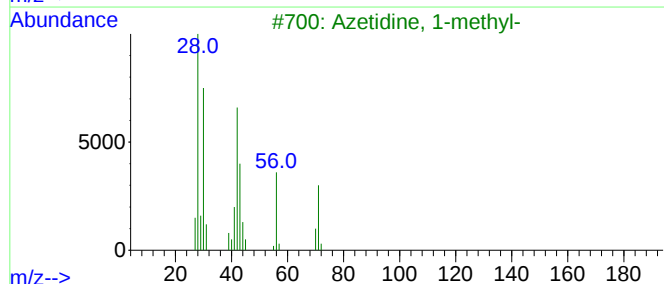
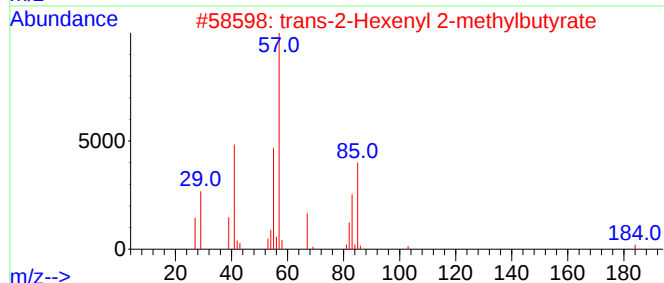
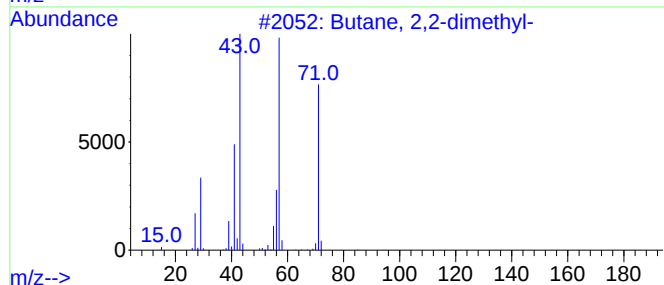
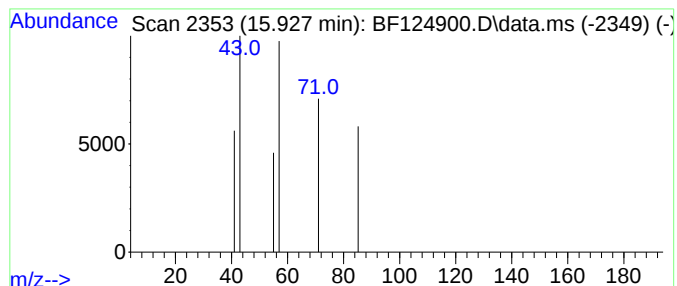
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown15.927 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.927	4.14 ng	5832	Perylene-d12	15.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	9
2			trans-2-Hexenyl 2-methylbutyrate	184	C11H20O2	1000433-23-8	9
3			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
4			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
5			1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080221\
Data File : BF124900.D
Acq On : 2 Aug 2021 10:55
Operator : JU/CG
Sample : M3228-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

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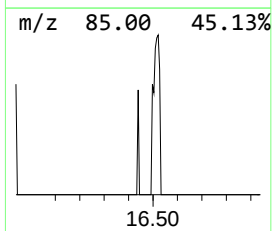
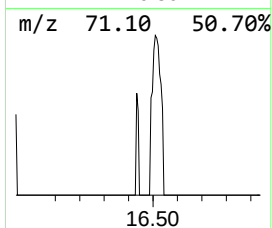
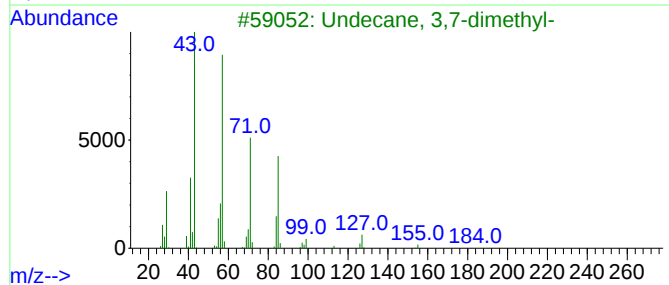
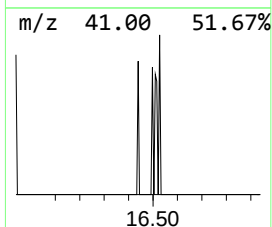
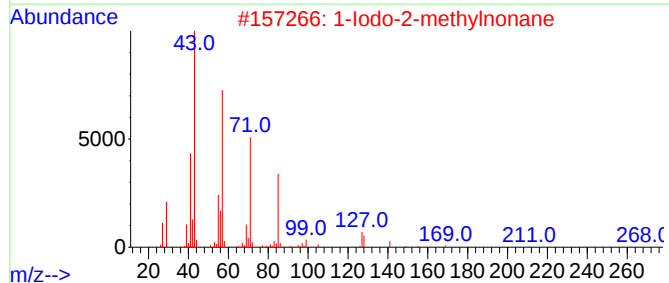
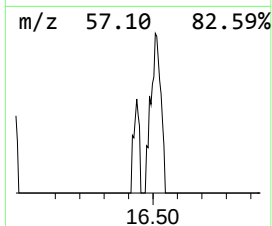
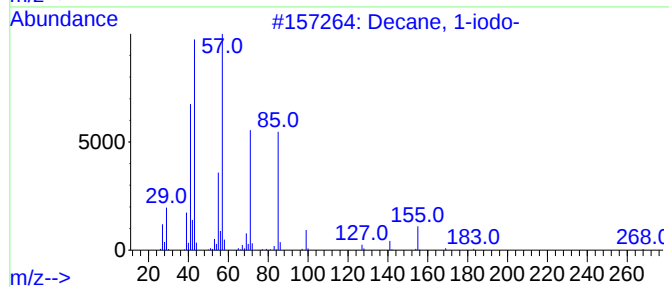
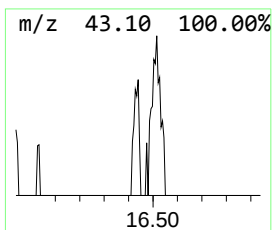
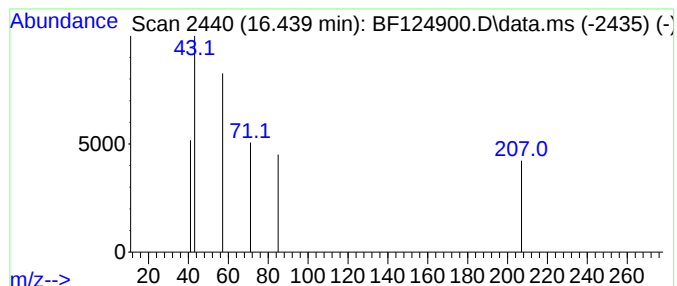
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown16.439 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.439	2.13 ng	3010	Perylene-d12	15.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 1-iodo-	268	C10H21I	002050-77-3	42
2			1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	36
3			Undecane, 3,7-dimethyl-	184	C13H28	017301-29-0	9
4			Decane, 2,3,7-trimethyl-	184	C13H28	062238-13-5	9
5			Undecane, 4-ethyl-	184	C13H28	017312-59-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080221\
Data File : BF124900.D
Acq On : 2 Aug 2021 10:55
Operator : JU/CG
Sample : M3228-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210552-COM-25

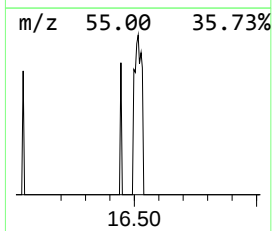
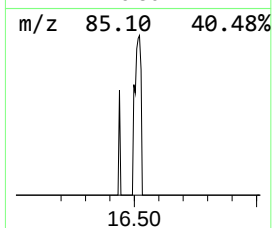
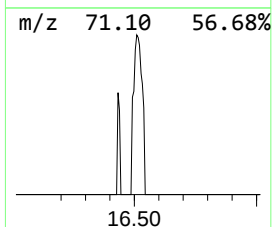
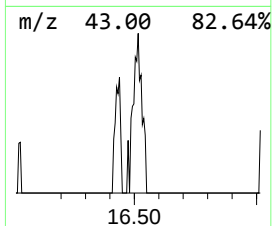
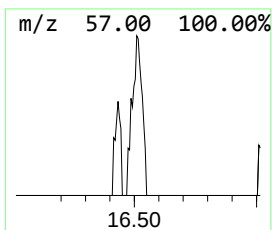
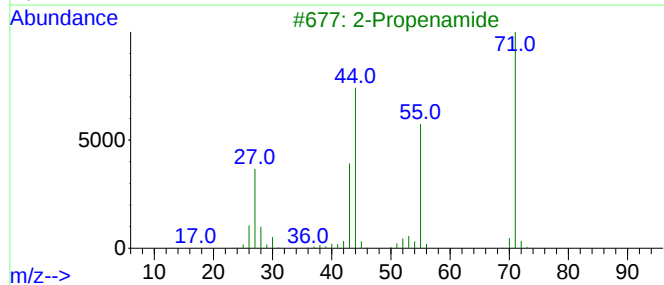
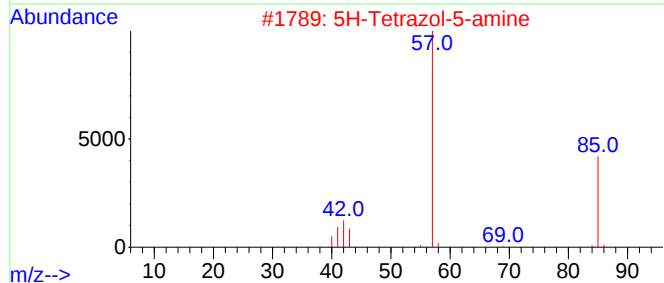
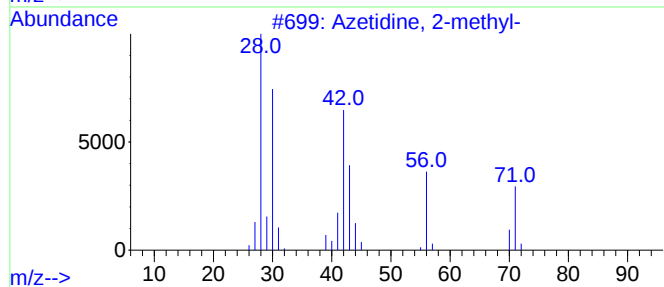
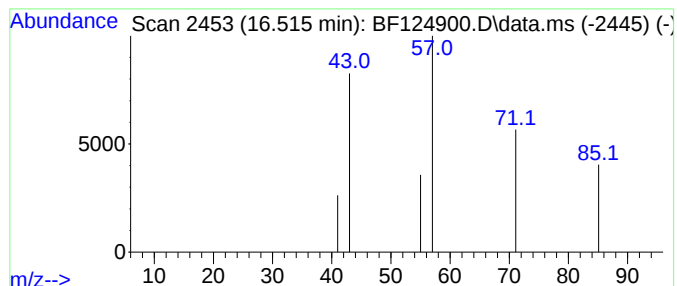
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown16.515 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.515	7.20 ng	10146	Perylene-d12	15.480

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
2		5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
3		2-Propenamide	71	C3H5NO	000079-06-1	4
4		1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
5		Oxalic acid, isohexyl neopentyl ...	244	C13H24O4	1000309-73-0	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080221\
Data File : BF124900.D
Acq On : 2 Aug 2021 10:55
Operator : JU/CG
Sample : M3228-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

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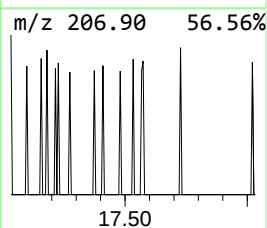
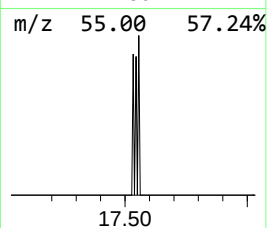
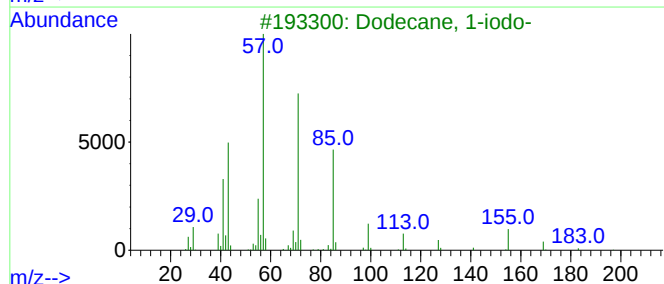
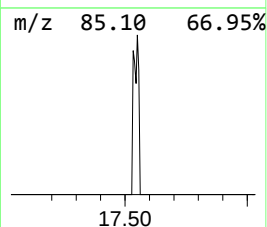
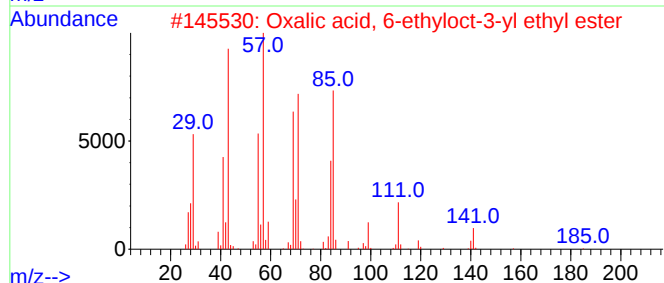
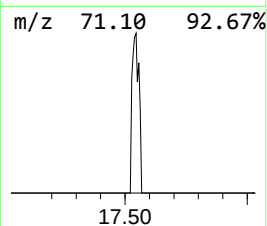
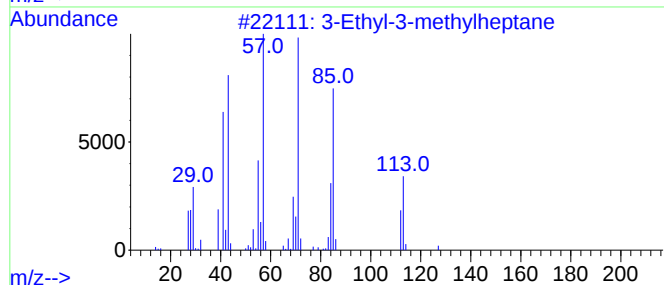
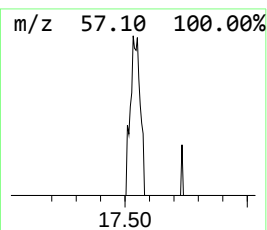
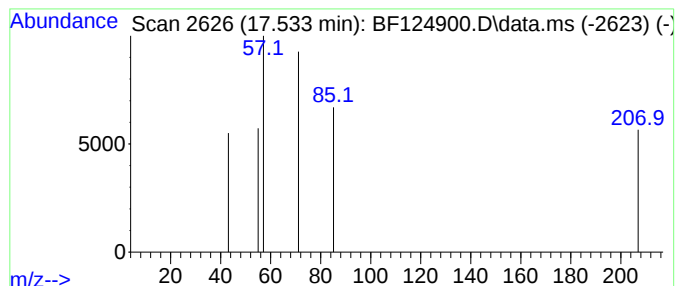
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown17.533 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.533	4.98 ng	7021	Perylene-d12	15.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Ethyl-3-methylheptane	142	C10H22	017302-01-1	38
2			Oxalic acid, 6-ethyloct-3-yl eth...	258	C14H26O4	1000309-33-9	9
3			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	9
4			Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	9
5			Pentanoic acid, 1,1-dimethylprop...	172	C10H20O2	117421-32-6	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080221\
Data File : BF124900.D
Acq On : 2 Aug 2021 10:55
Operator : JU/CG
Sample : M3228-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210552-COM-25

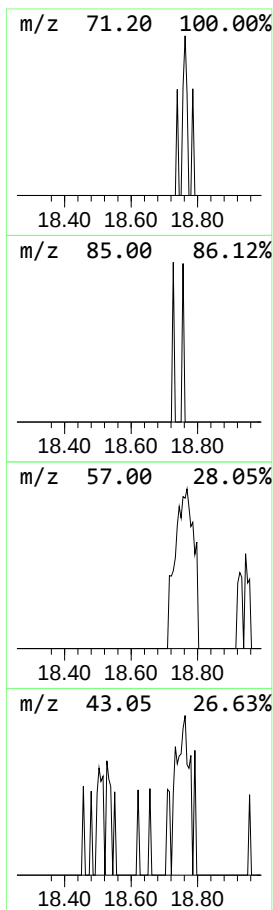
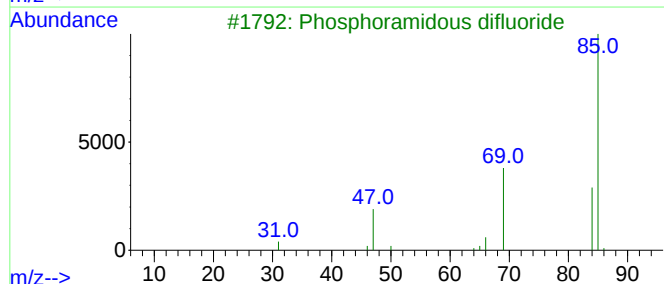
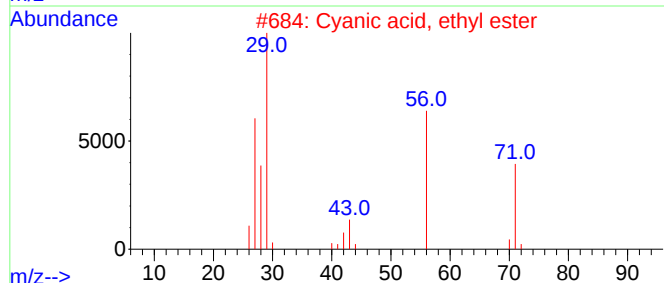
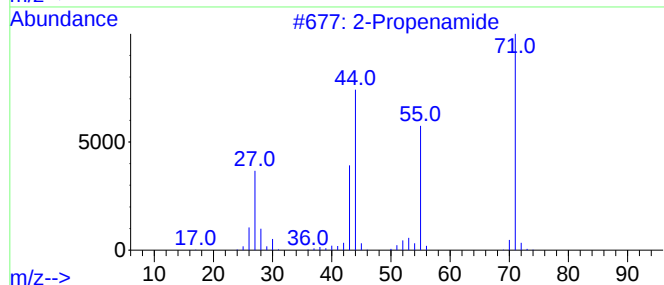
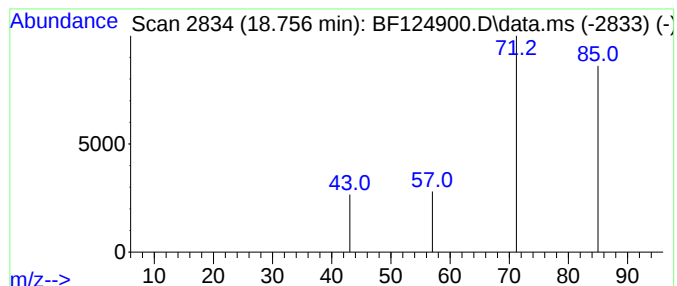
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown18.756 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.756	2.49 ng	3508	Perylene-d12	15.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propenamide	71	C3H5NO	000079-06-1	4
2			Cyanoic acid, ethyl ester	71	C3H5NO	000627-48-5	3
3			Phosphoramidous difluoride	85	F2H2NP	025757-74-8	2
4			3H-1,2,4-Triazol-3-one, 1,2-dihy...	85	C2H3N3O	000930-33-6	2
5			Isothiazole	85	C3H3NS	000288-16-4	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080221\
Data File : BF124900.D
Acq On : 2 Aug 2021 10:55
Operator : JU/CG
Sample : M3228-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210552-COM-25

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
Decanoic acid, ...	11.892	18.9	ng	43396	4	11.374	45955	20.0
Octadecanoic acid	12.680	20.0	ng	45904	4	11.374	45955	20.0
Nonadecane	13.327	30.1	ng	51564	5	14.010	34233	20.0
Heptacosane	14.216	21.5	ng	36838	5	14.010	34233	20.0
unknown14.892	14.892	14.5	ng	20389	6	15.480	28201	20.0
unknown15.116	15.116	4.0	ng	5564	6	15.480	28201	20.0
unknown15.351	15.351	2.3	ng	3237	6	15.480	28201	20.0
unknown15.645	15.645	9.1	ng	12842	6	15.480	28201	20.0
unknown15.927	15.927	4.1	ng	5832	6	15.480	28201	20.0
unknown16.439	16.439	2.1	ng	3010	6	15.480	28201	20.0
unknown16.515	16.515	7.2	ng	10146	6	15.480	28201	20.0
unknown17.533	17.533	5.0	ng	7021	6	15.480	28201	20.0
unknown18.756	18.756	2.5	ng	3508	6	15.480	28201	20.0