

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053023\
 Data File : BF133528.D
 Acq On : 30 May 2023 18:22
 Operator : CG\JU
 Sample : 02955-09
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DUP03

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-BF052523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133528.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	14	rVB	236027	298191	7.90%	1.051%
2	5.057	498	505	515	rVB	153508	201888	5.35%	0.711%
3	5.451	566	572	575	rBV	3064505	3383229	89.58%	11.920%
4	6.457	737	743	746	rBV	3110564	3476943	92.06%	12.250%
5	6.828	803	806	810	rBV	1009889	879077	23.28%	3.097%
6	7.398	897	903	905	rBV	2191881	2205530	58.40%	7.771%
7	8.116	1021	1025	1028	rBV	1294877	1151027	30.48%	4.055%
8	9.192	1203	1208	1211	rBV	4399665	3753672	99.39%	13.225%
9	9.869	1319	1323	1326	rBV	1557096	1223877	32.41%	4.312%
10	10.580	1441	1444	1448	rBV	213884	185147	4.90%	0.652%
11	10.657	1452	1457	1460	rBV	2745261	2455828	65.03%	8.652%
12	11.357	1572	1576	1579	rBV	1468935	1316741	34.87%	4.639%
13	11.886	1662	1666	1670	rBV	224490	210757	5.58%	0.743%
14	12.563	1778	1781	1785	rBV	112443	109258	2.89%	0.385%
15	12.668	1796	1799	1805	rBV2	39310	42478	1.12%	0.150%
16	12.792	1814	1820	1823	rBV	103208	107182	2.84%	0.378%
17	12.945	1842	1846	1850	rVB	3652527	3776624	100.00%	13.306%
18	13.121	1869	1876	1879	rBV2	25212	44709	1.18%	0.158%
19	13.180	1879	1886	1890	rBV2	78548	152016	4.03%	0.536%
20	13.521	1941	1944	1952	rVB	130638	112315	2.97%	0.396%
21	13.851	1996	2000	2013	rVB	301948	391131	10.36%	1.378%
22	13.998	2020	2025	2027	rBV	1119260	1116553	29.56%	3.934%
23	14.015	2027	2028	2035	rVB	52885	48256	1.28%	0.170%
24	14.168	2051	2054	2059	rBV	177681	155581	4.12%	0.548%
25	14.474	2103	2106	2110	rBV	165084	154100	4.08%	0.543%
26	14.780	2155	2158	2163	rBV	100892	103431	2.74%	0.364%
27	15.027	2196	2200	2208	rVB	40434	78803	2.09%	0.278%
28	15.121	2212	2216	2220	rVV2	85238	97918	2.59%	0.345%
29	15.386	2257	2261	2267	rVB	33908	44506	1.18%	0.157%
30	15.451	2267	2272	2277	rBV	647850	784870	20.78%	2.765%
31	15.498	2277	2280	2285	rVB	53874	69332	1.84%	0.244%
32	15.939	2350	2355	2359	rBV	50941	70695	1.87%	0.249%
33	16.445	2436	2441	2447	rVB2	36452	65860	1.74%	0.232%
34	17.039	2536	2542	2553	rBV3	26919	61579	1.63%	0.217%
35	17.745	2657	2662	2675	rVB6	21488	54022	1.43%	0.190%

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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-BF052523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

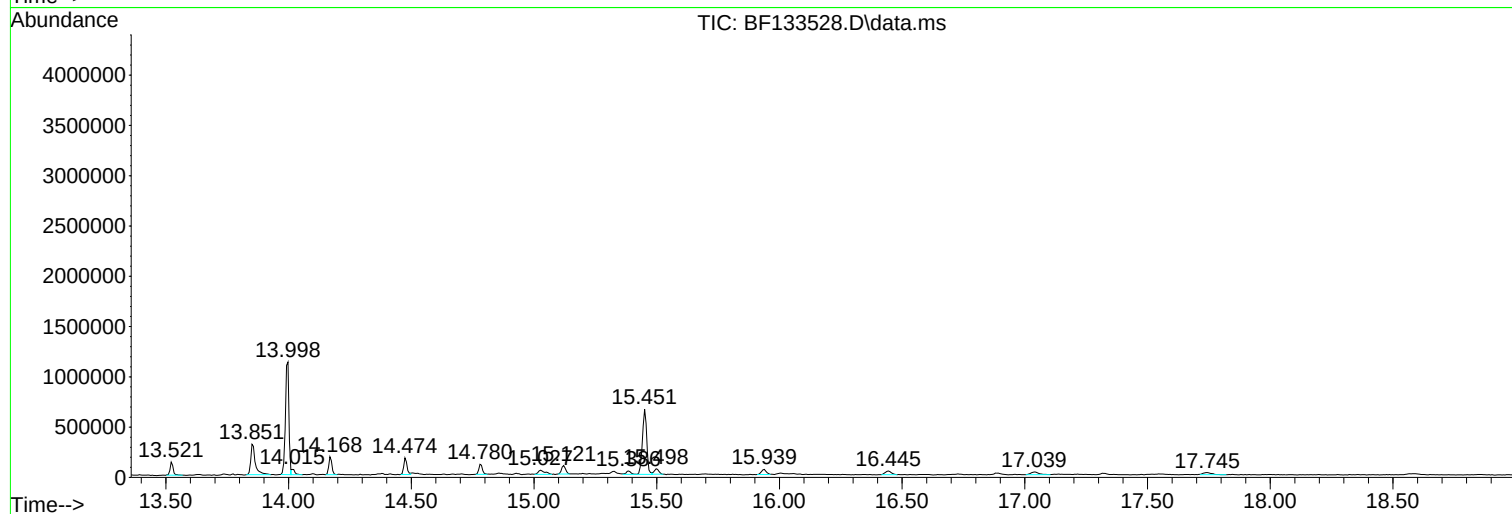
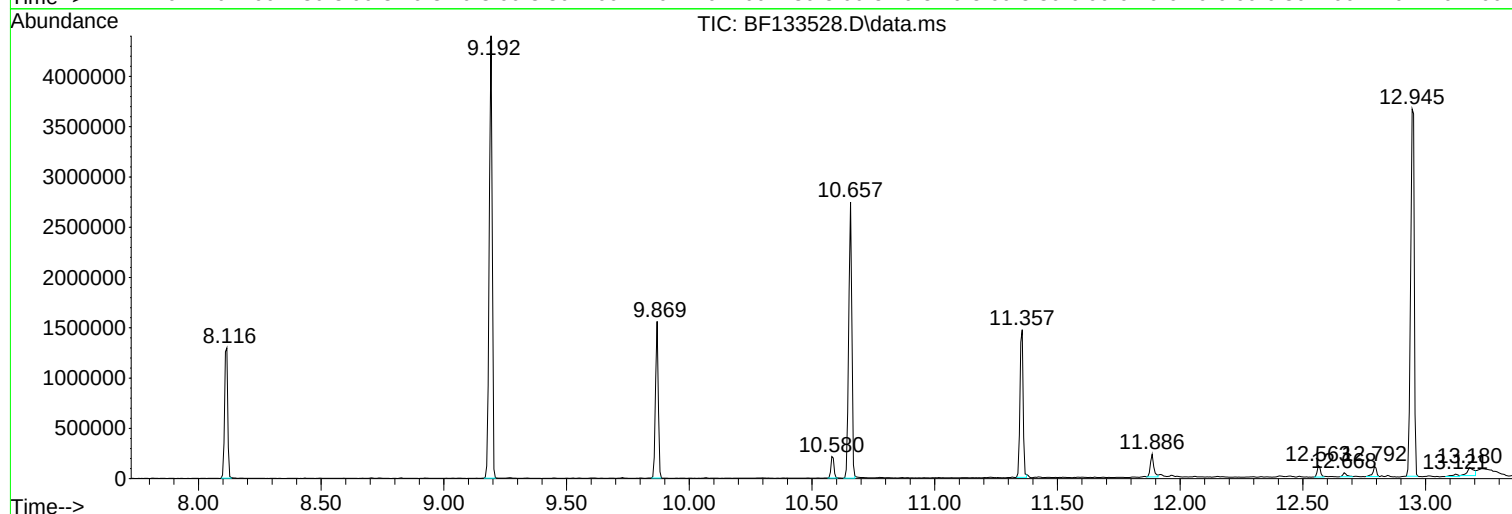
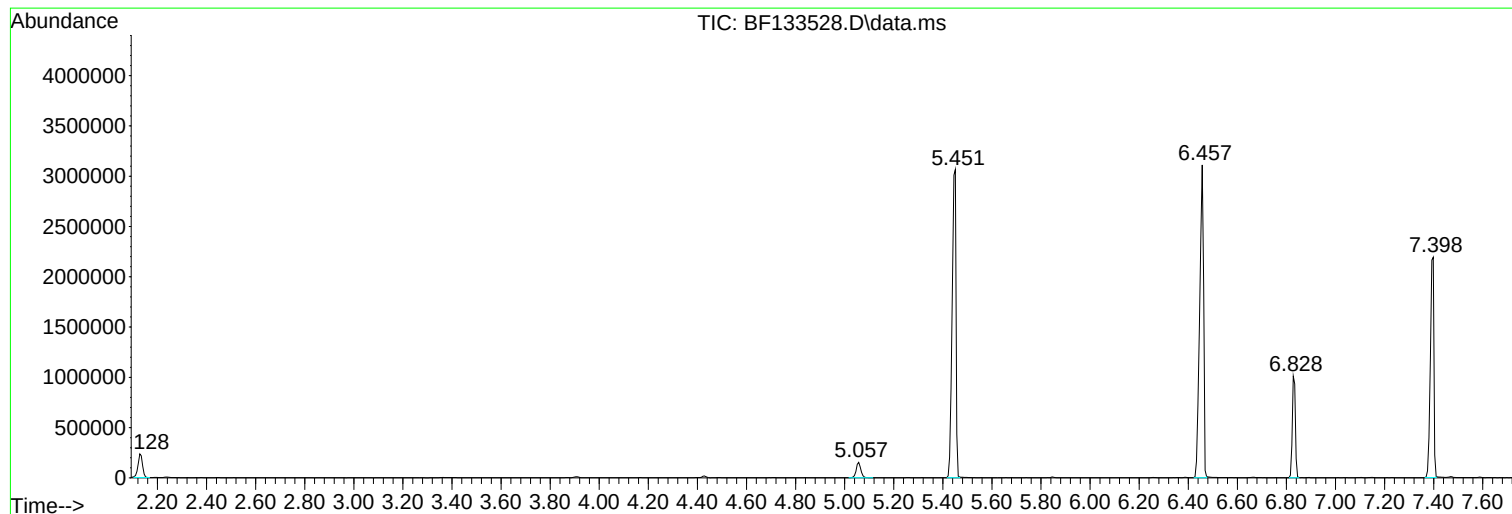
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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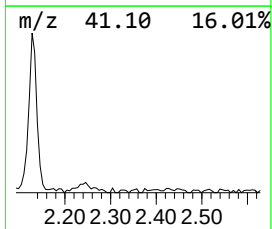
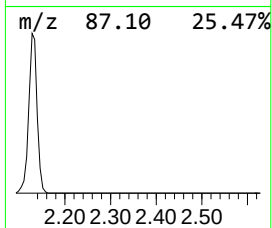
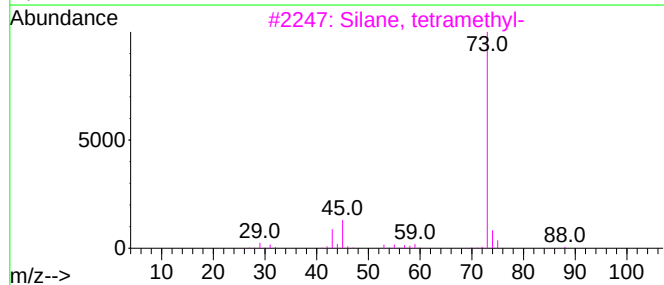
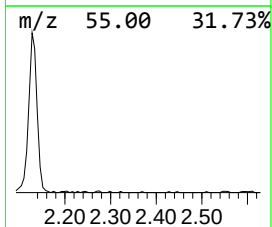
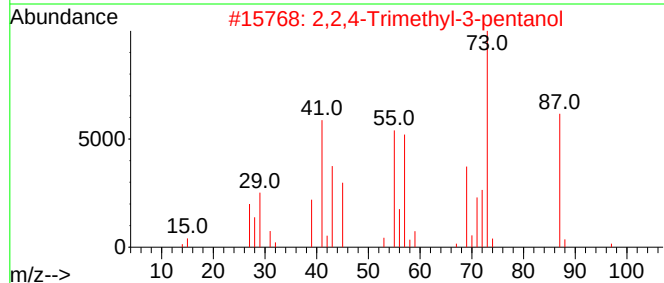
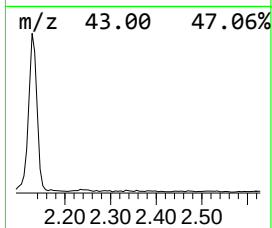
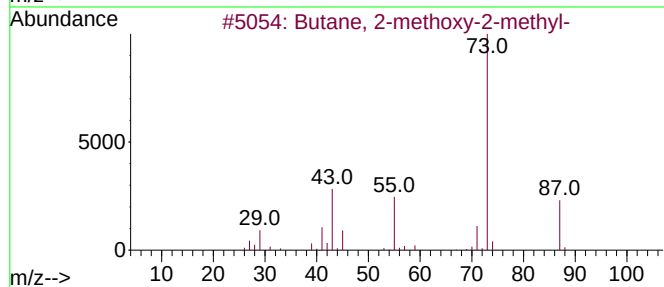
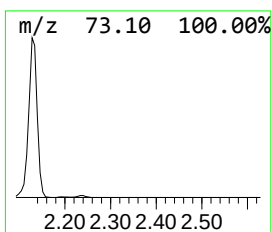
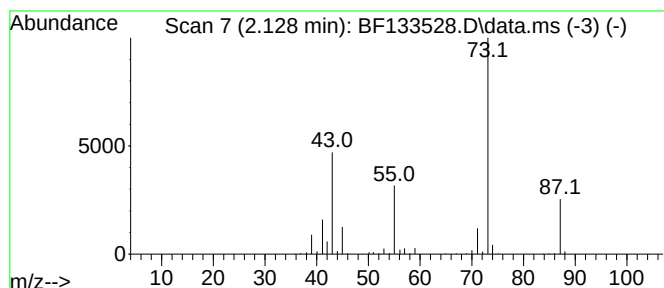
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	6.78 ng	298191	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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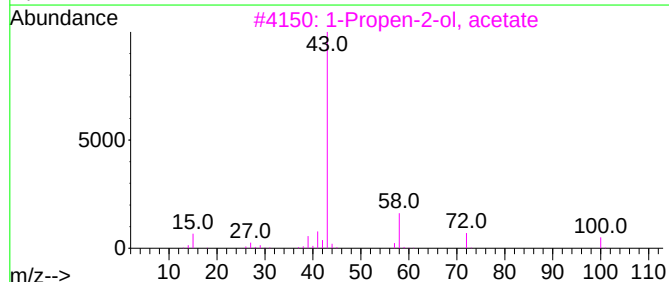
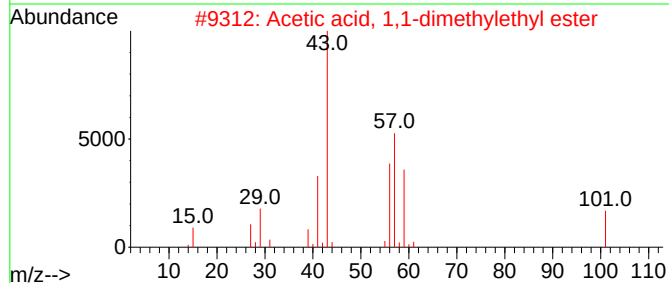
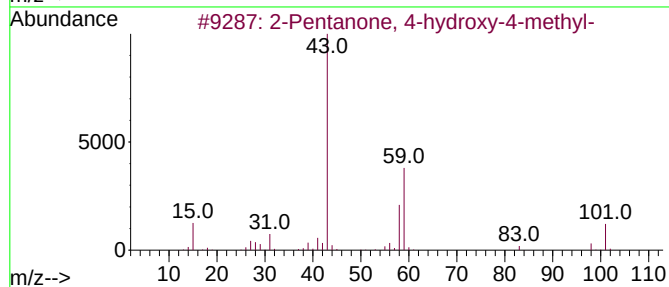
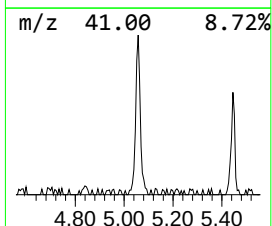
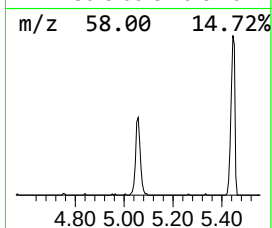
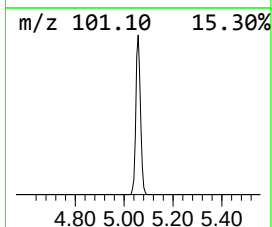
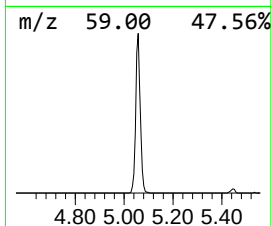
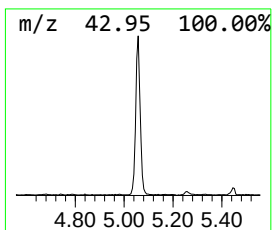
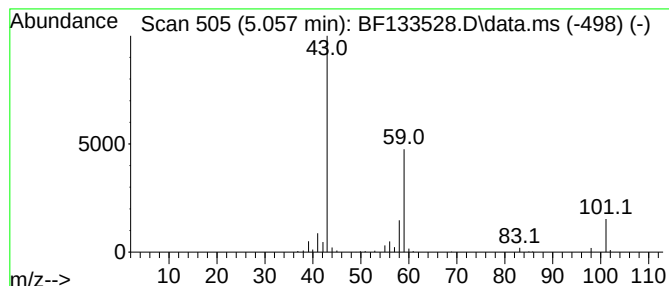
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	4.59 ng	201888	1,4-Dichlorobenzene-d4	6.834

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		3,3-Dimethylbutylamine	101	C6H15N	015673-00-4	9
5		2-Pentanone	86	C5H10O	000107-87-9	9



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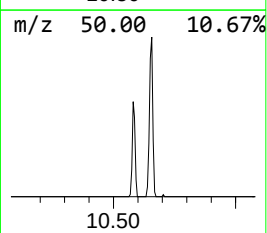
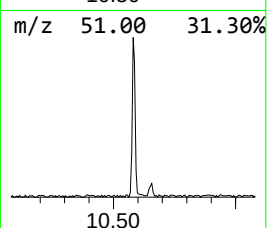
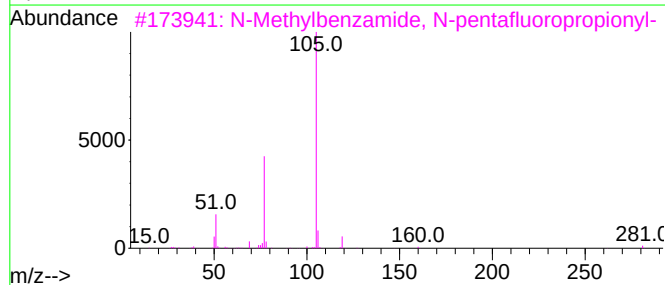
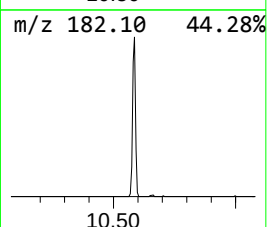
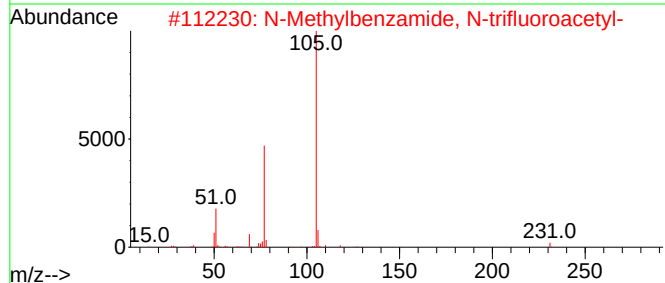
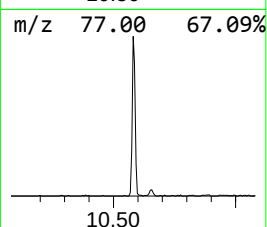
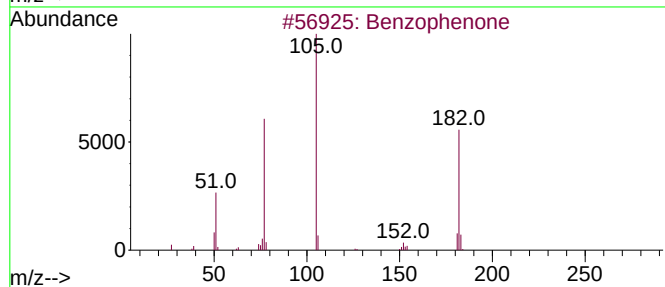
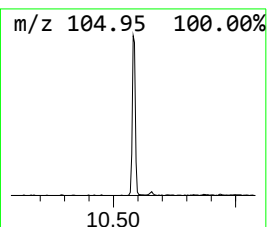
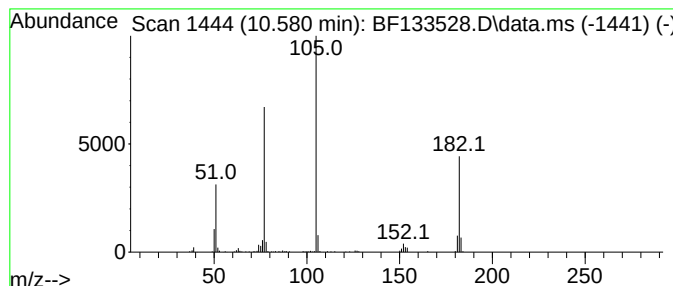
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.580	3.03 ng	185147	Acenaphthene-d10	9.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	50
3			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	50
4			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	50
5			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50



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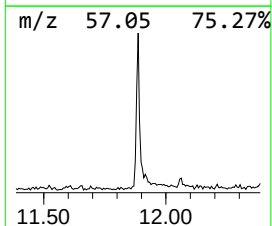
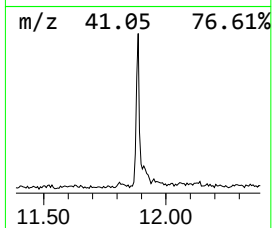
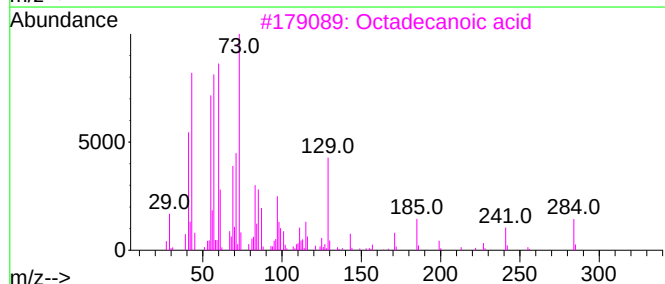
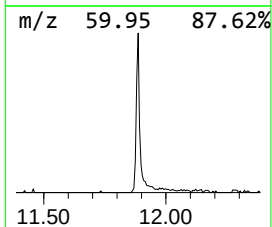
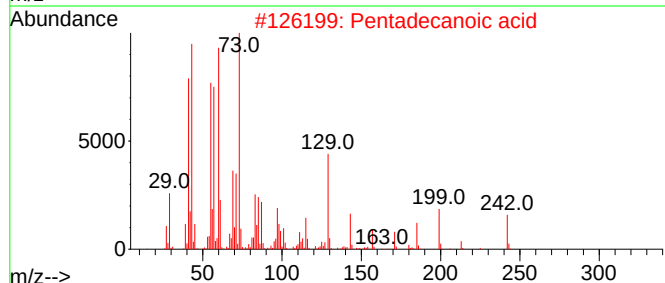
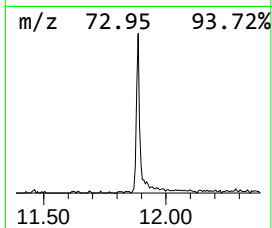
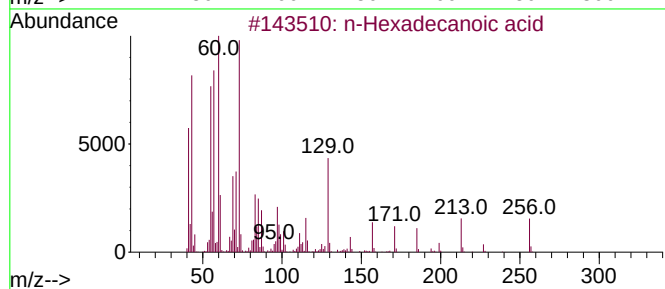
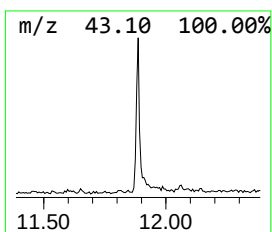
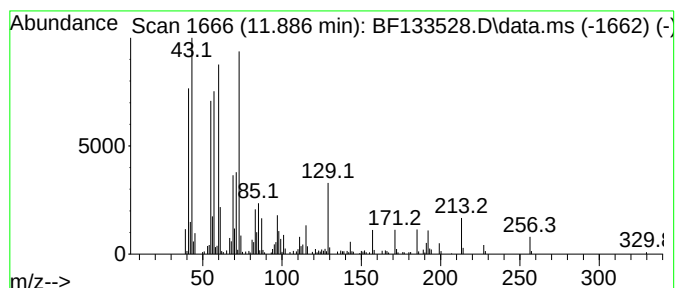
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.886	3.20 ng	210757	Phenanthrene-d10	11.357	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Octadecanoic acid	284	C18H36O2	000057-11-4	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	76



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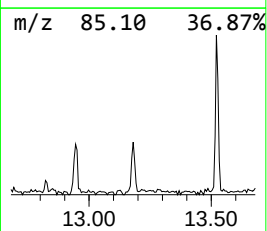
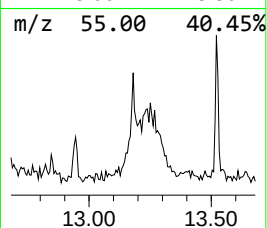
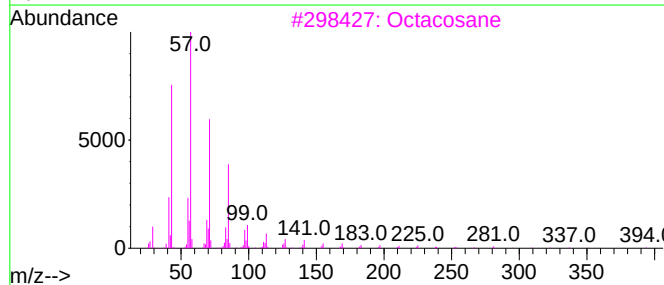
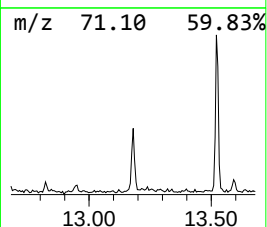
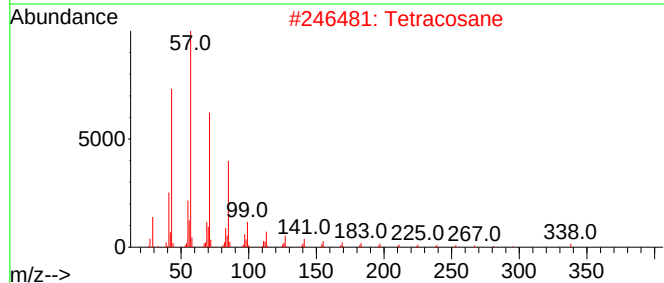
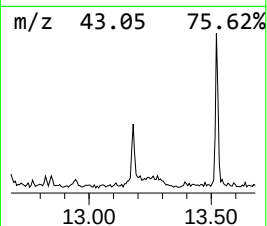
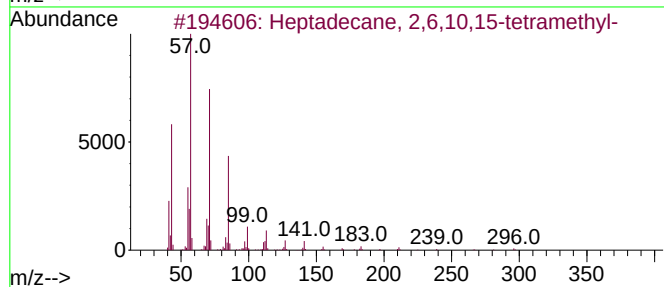
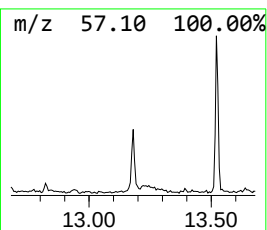
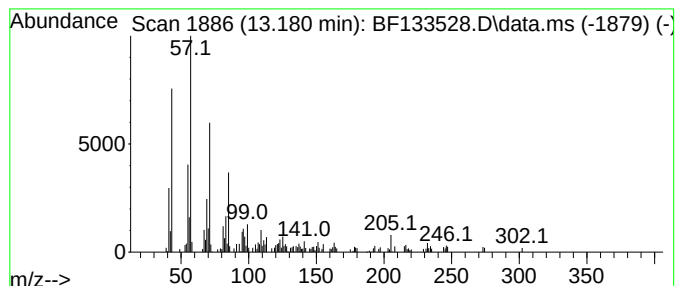
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heptadecane, 2,6,10,15-tetr... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.180	2.72 ng	152016	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	62
2			Tetracosane	338	C24H50	000646-31-1	62
3			Octacosane	394	C28H58	000630-02-4	62
4			Eicosane	282	C20H42	000112-95-8	62
5			Nonadecane	268	C19H40	000629-92-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053023\
Data File : BF133528.D
Acq On : 30 May 2023 18:22
Operator : CG\JU
Sample : 02955-09
Misc :
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Instrument :
BNA_F
ClientSampleId :
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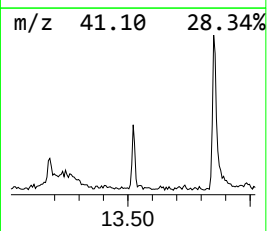
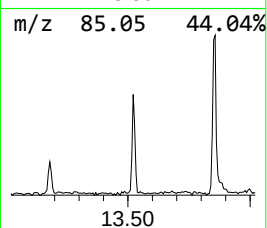
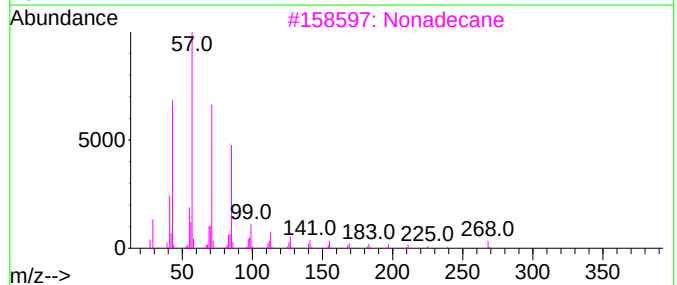
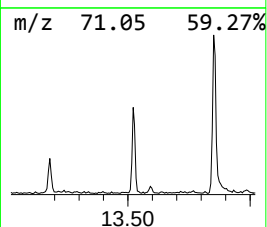
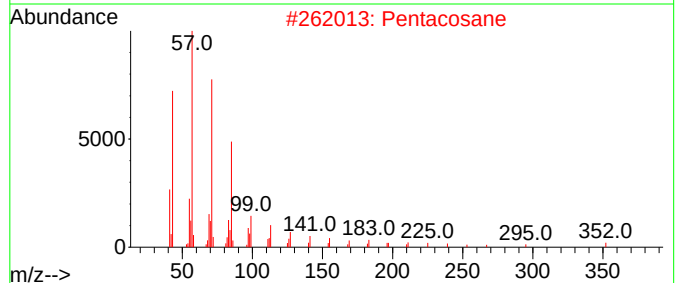
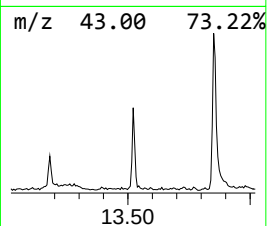
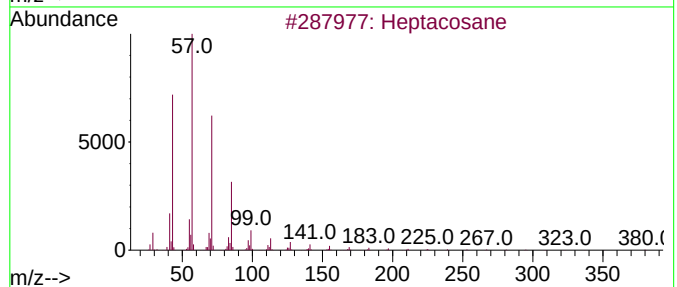
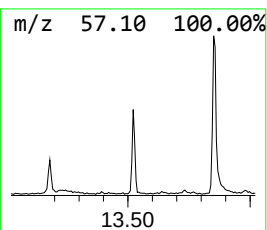
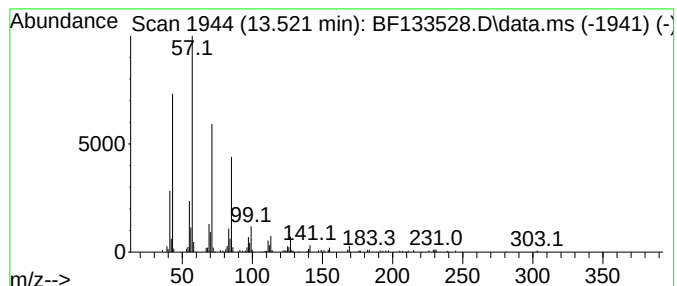
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.521	2.01 ng	112315	Chrysene-d12	13.998

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	91
2		Pentacosane	352	C25H52	000629-99-2	90
3		Nonadecane	268	C19H40	000629-92-5	90
4		Hexadecane	226	C16H34	000544-76-3	87
5		Tetradecane	198	C14H30	000629-59-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053023\
Data File : BF133528.D
Acq On : 30 May 2023 18:22
Operator : CG\JU
Sample : 02955-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

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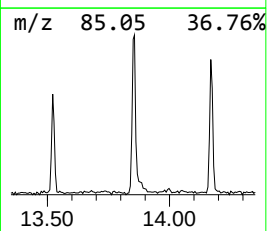
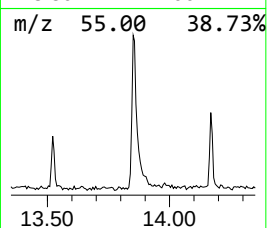
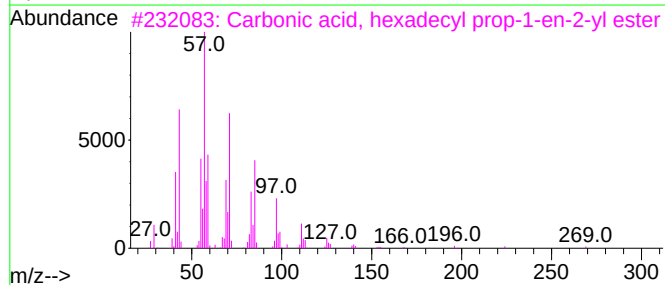
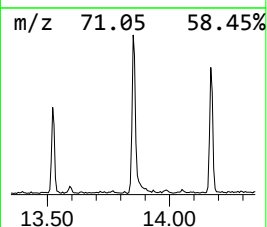
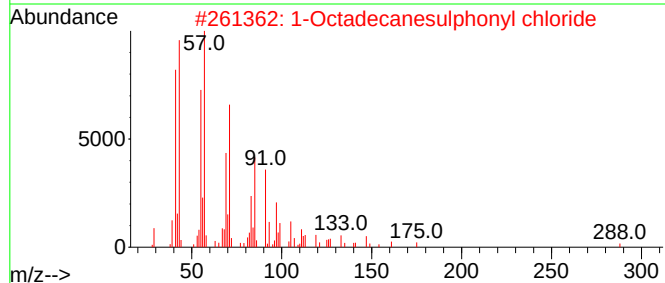
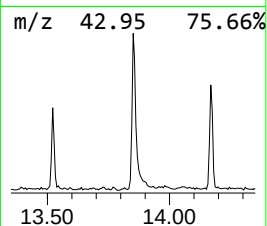
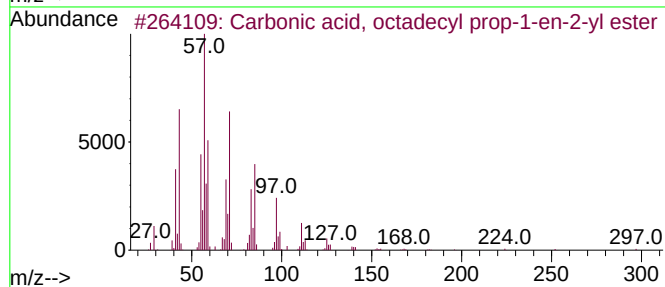
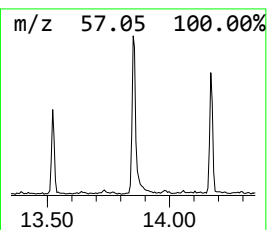
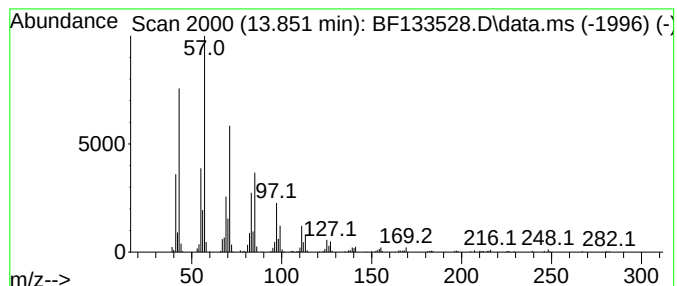
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Carbonic acid, octadecyl pr... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	7.01 ng	391131	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	91
2			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	91
3			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	91
4			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	90
5			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053023\
Data File : BF133528.D
Acq On : 30 May 2023 18:22
Operator : CG\JU
Sample : 02955-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

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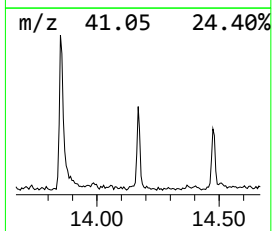
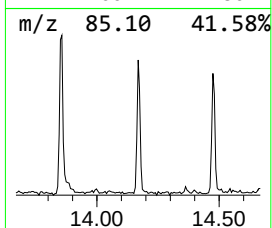
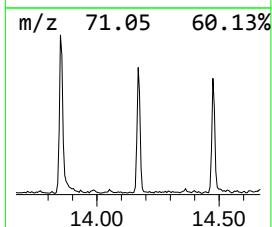
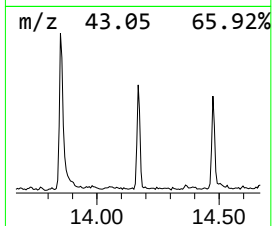
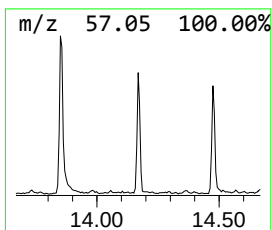
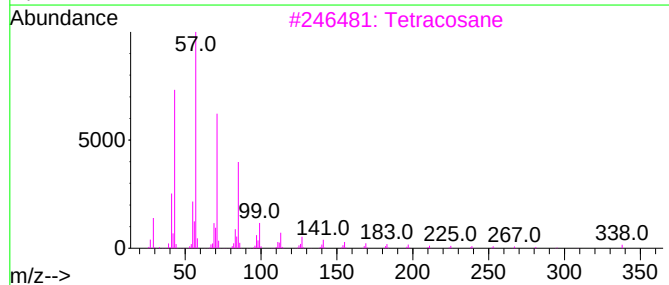
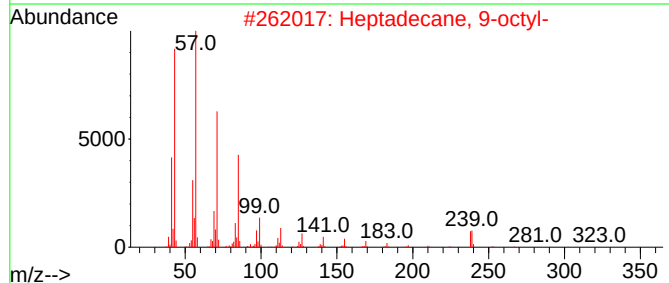
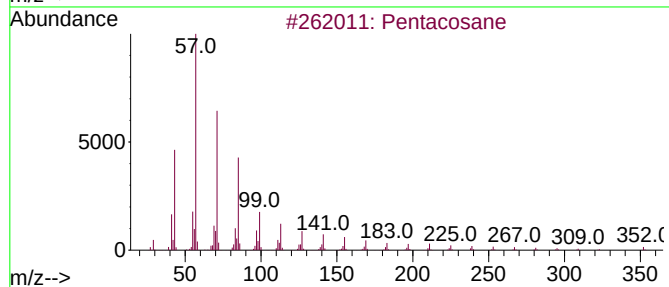
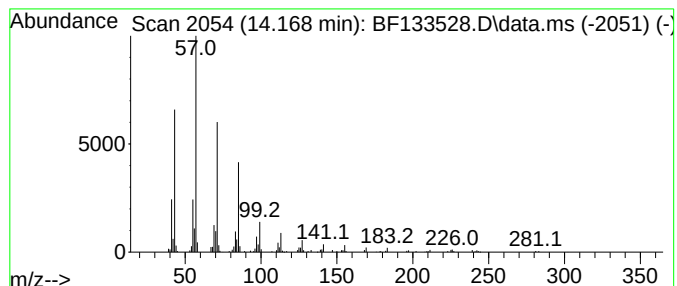
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.168	2.79 ng	155581	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	91
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3			Tetracosane	338	C24H50	000646-31-1	91
4			Heptacosane	380	C27H56	000593-49-7	91
5			Tetratetracontane	619	C44H90	007098-22-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053023\
Data File : BF133528.D
Acq On : 30 May 2023 18:22
Operator : CG\JU
Sample : 02955-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP03

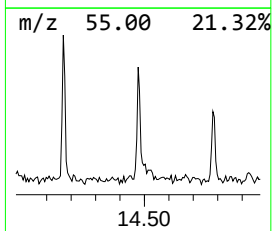
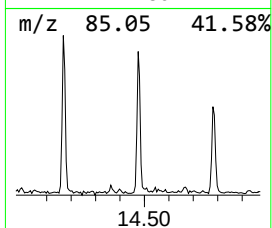
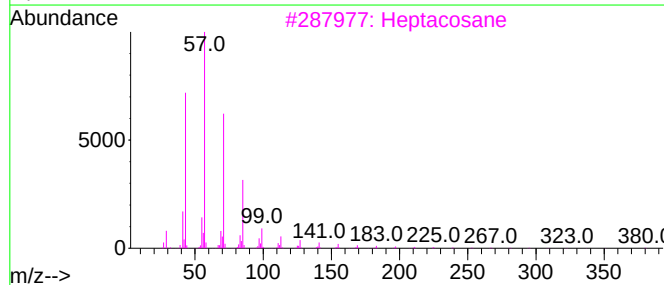
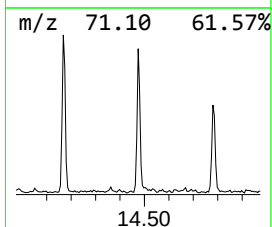
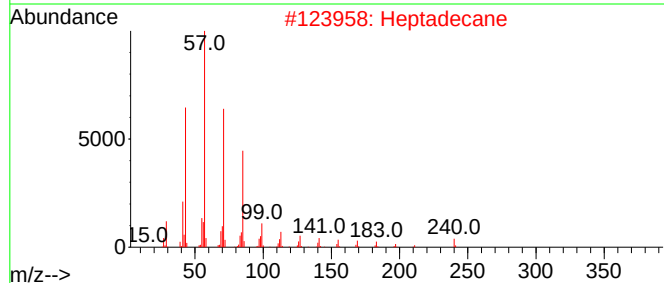
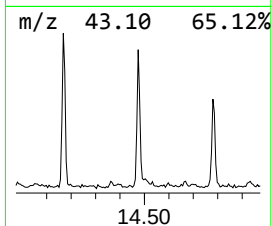
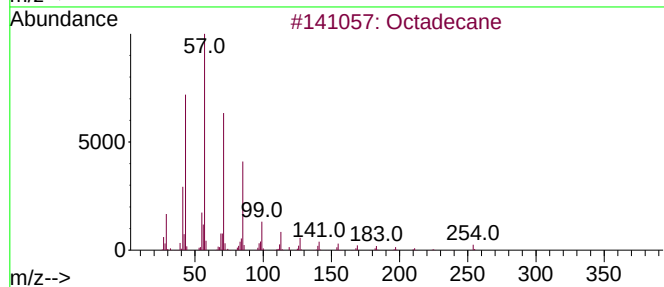
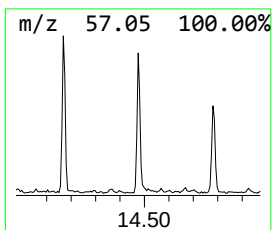
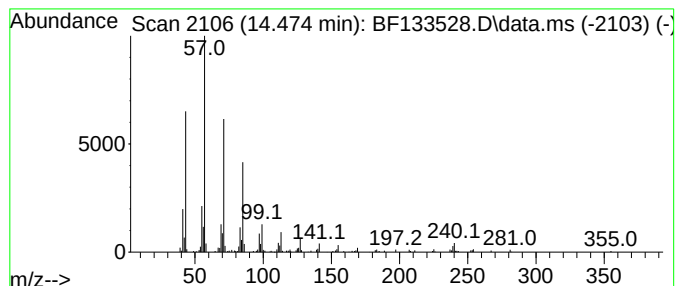
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.474	2.76 ng	154100	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	97
2			Heptadecane	240	C17H36	000629-78-7	94
3			Heptacosane	380	C27H56	000593-49-7	90
4			Heneicosane	296	C21H44	000629-94-7	90
5			Octacosane	394	C28H58	000630-02-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053023\
Data File : BF133528.D
Acq On : 30 May 2023 18:22
Operator : CG\JU
Sample : 02955-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

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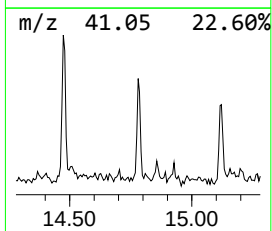
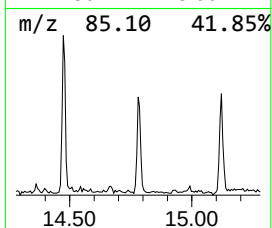
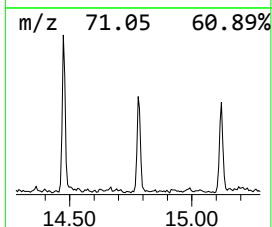
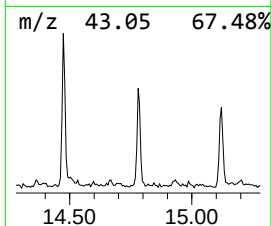
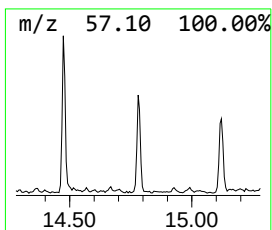
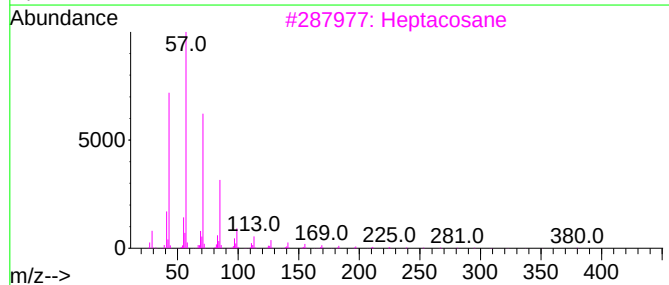
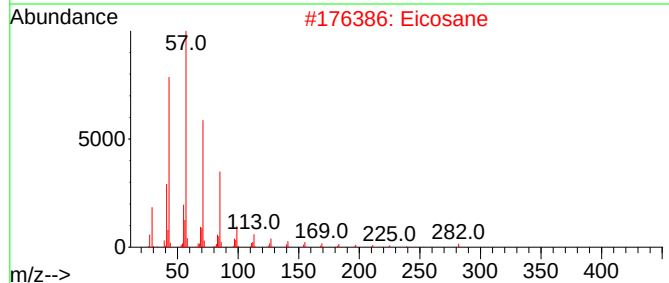
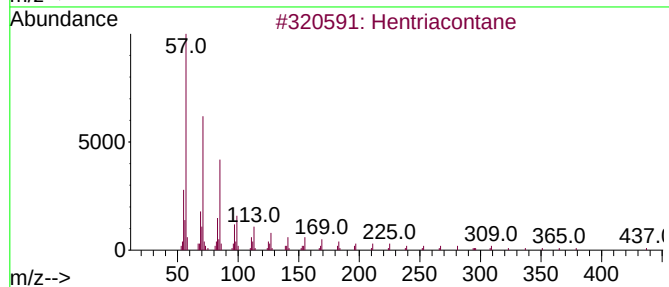
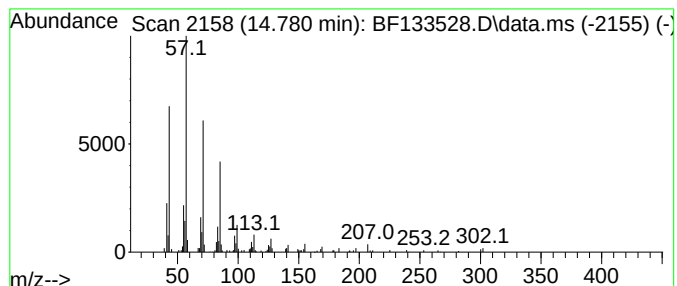
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hentriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	2.64 ng	103431	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	90
2			Eicosane	282	C20H42	000112-95-8	90
3			Heptacosane	380	C27H56	000593-49-7	90
4			Octacosane	394	C28H58	000630-02-4	90
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053023\
Data File : BF133528.D
Acq On : 30 May 2023 18:22
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Sample : 02955-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

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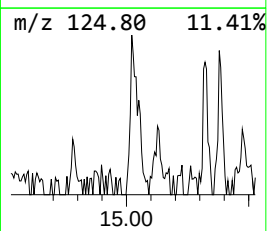
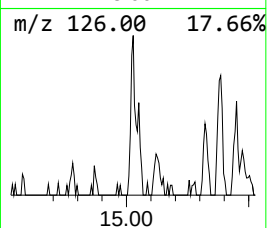
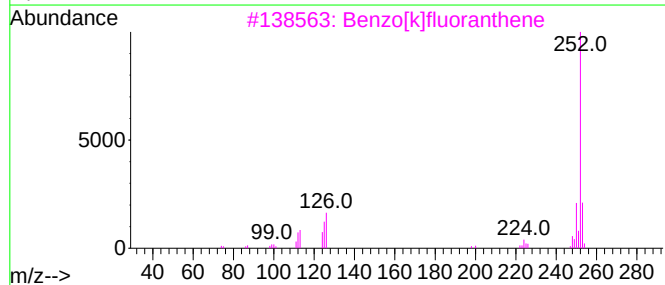
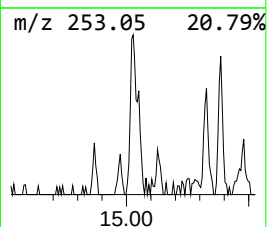
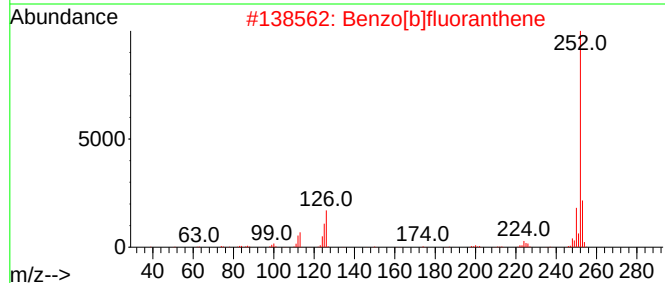
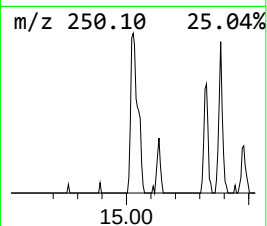
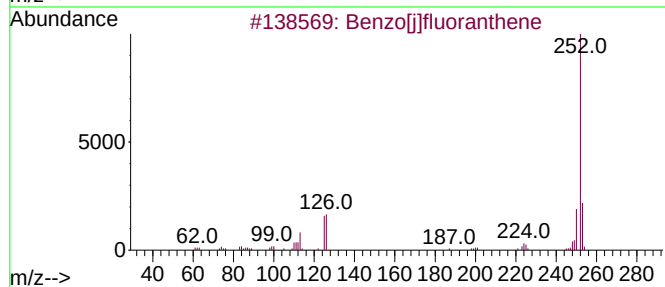
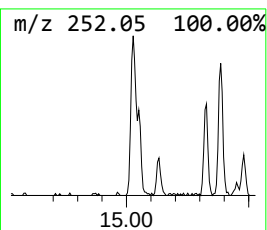
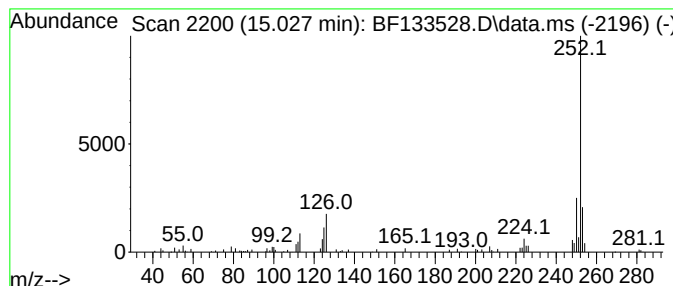
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzo[j]fluoranthene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.027	2.01 ng	78803	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[j]fluoranthene	252	C20H12	000205-82-3	96
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4			Benzo[a]pyrene	252	C20H12	000050-32-8	94
5			Benzo[e]pyrene	252	C20H12	000192-97-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053023\
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Acq On : 30 May 2023 18:22
Operator : CG\JU
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Misc :
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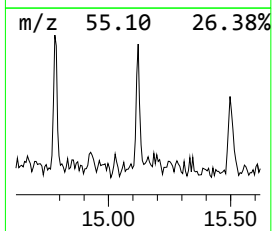
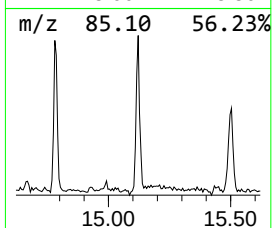
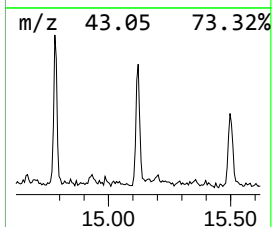
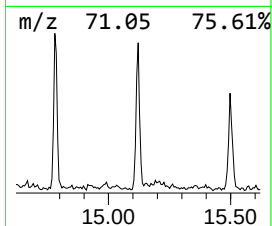
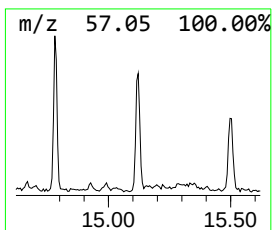
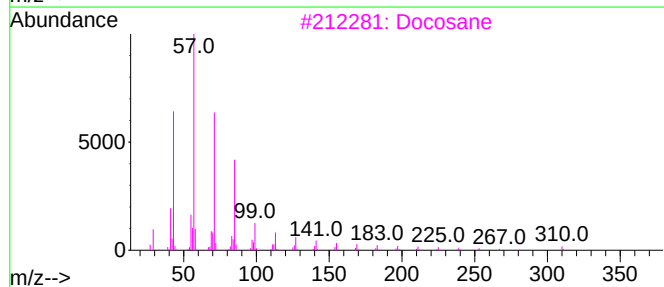
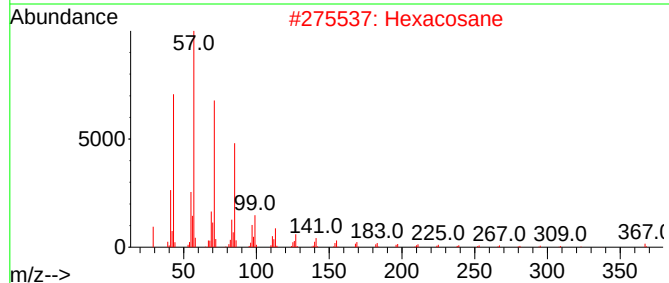
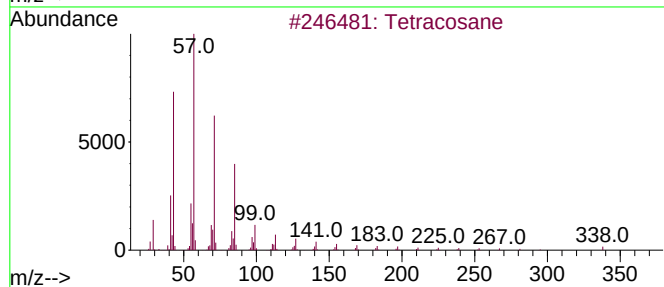
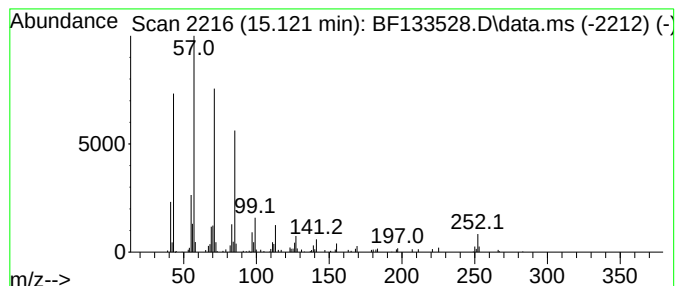
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tetracosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.121	2.50 ng	97918	Perylene-d12	15.451	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	90
2	Hexacosane	366	C26H54	000630-01-3	90
3	Docosane	310	C22H46	000629-97-0	87
4	Heptacosane	380	C27H56	000593-49-7	87
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053023\
Data File : BF133528.D
Acq On : 30 May 2023 18:22
Operator : CG\JU
Sample : 02955-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.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	6.8	ng	298191	1	6.834	879077	20.0
2-Pentanone, 4-...	5.057	4.6	ng	201888	1	6.834	879077	20.0
Benzophenone	10.580	3.0	ng	185147	3	9.869	1223880	20.0
n-Hexadecanoic ...	11.886	3.2	ng	210757	4	11.357	1316740	20.0
Heptadecane, 2,...	13.180	2.7	ng	152016	5	13.998	1116550	20.0
Heptacosane	13.521	2.0	ng	112315	5	13.998	1116550	20.0
Carbonic acid, ...	13.851	7.0	ng	391131	5	13.998	1116550	20.0
Pentacosane	14.168	2.8	ng	155581	5	13.998	1116550	20.0
Octadecane	14.474	2.8	ng	154100	5	13.998	1116550	20.0
Hentriacontane	14.780	2.6	ng	103431	6	15.451	784870	20.0
Benzo[j]fluoran...	15.027	2.0	ng	78803	6	15.451	784870	20.0
Tetracosane	15.121	2.5	ng	97918	6	15.451	784870	20.0