

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
 Data File : BF122185.D
 Acq On : 30 Oct 2020 17:42
 Operator : JU/CG
 Sample : L4532-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 IB1-TREATED-EFFLU

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-BF101220.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122185.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.339	550	553	589	rBV	1059777	1705947	47.60%	6.853%
2	6.369	725	728	755	rBV	684010	1169066	32.62%	4.696%
3	6.710	783	786	797	rVB	653203	626093	17.47%	2.515%
4	7.281	879	883	904	rBV	1903194	2137381	59.64%	8.586%
5	7.928	990	993	1001	rBV	49890	108534	3.03%	0.436%
6	7.992	1001	1004	1020	rVB	851991	868508	24.23%	3.489%
7	9.069	1182	1187	1190	rBV	3790568	3527289	98.42%	14.169%
8	9.469	1252	1255	1264	rBV	346199	327066	9.13%	1.314%
9	9.745	1298	1302	1309	rBV	1104355	975881	27.23%	3.920%
10	10.145	1366	1370	1372	rBV	258481	220801	6.16%	0.887%
11	10.169	1372	1374	1377	rVB	62877	48797	1.36%	0.196%
12	10.539	1433	1437	1452	rBV	2411455	2512589	70.10%	10.093%
13	11.233	1552	1555	1566	rBV	1074565	1030605	28.76%	4.140%
14	11.768	1641	1646	1660	rBV	672230	805238	22.47%	3.235%
15	12.457	1759	1763	1764	rBV2	46182	52472	1.46%	0.211%
16	12.551	1775	1779	1791	rBV	396838	478884	13.36%	1.924%
17	12.704	1803	1805	1813	rVB3	30764	38443	1.07%	0.154%
18	12.821	1820	1825	1828	rBV	3722031	3584089	100.00%	14.397%
19	13.039	1857	1862	1867	rBV	59596	67785	1.89%	0.272%
20	13.380	1917	1920	1922	rBV	89031	83986	2.34%	0.337%
21	13.492	1936	1939	1947	rVB	61614	67557	1.88%	0.271%
22	13.710	1972	1976	1991	rBV	424328	561172	15.66%	2.254%
23	13.880	2002	2005	2017	rVB	791798	849981	23.72%	3.414%
24	14.021	2026	2029	2032	rBV	102037	88665	2.47%	0.356%
25	14.204	2056	2060	2064	rBV4	50091	54209	1.51%	0.218%
26	14.327	2077	2081	2084	rBV	114149	109789	3.06%	0.441%
27	14.457	2099	2103	2105	rBV	38069	39464	1.10%	0.159%
28	14.486	2105	2108	2111	rVB	77209	69528	1.94%	0.279%
29	14.621	2127	2131	2135	rBV	98639	97070	2.71%	0.390%
30	14.692	2138	2143	2149	rBV	194822	190406	5.31%	0.765%
31	14.921	2178	2182	2183	rBV	80588	89492	2.50%	0.359%
32	14.939	2183	2185	2196	rVB2	141420	207560	5.79%	0.834%
33	15.268	2239	2241	2243	rBV	64663	75067	2.09%	0.302%
34	15.321	2247	2250	2264	rVB	456531	649693	18.13%	2.610%
35	15.698	2309	2314	2318	rBV	90205	126515	3.53%	0.508%
36	16.162	2388	2393	2398	rBV	86664	137715	3.84%	0.553%

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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-BF101220.M
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37	16.703	2479	2485	2487	rBV2	58762	103197	2.88%	0.415%
38	16.745	2487	2492	2504	rVB	192602	438229	12.23%	1.760%
39	17.174	2560	2565	2585	rBV2	108736	350380	9.78%	1.407%
40	17.345	2588	2594	2605	rVB2	54801	135954	3.79%	0.546%
41	18.103	2716	2723	2733	rVB3	31394	84017	2.34%	0.337%

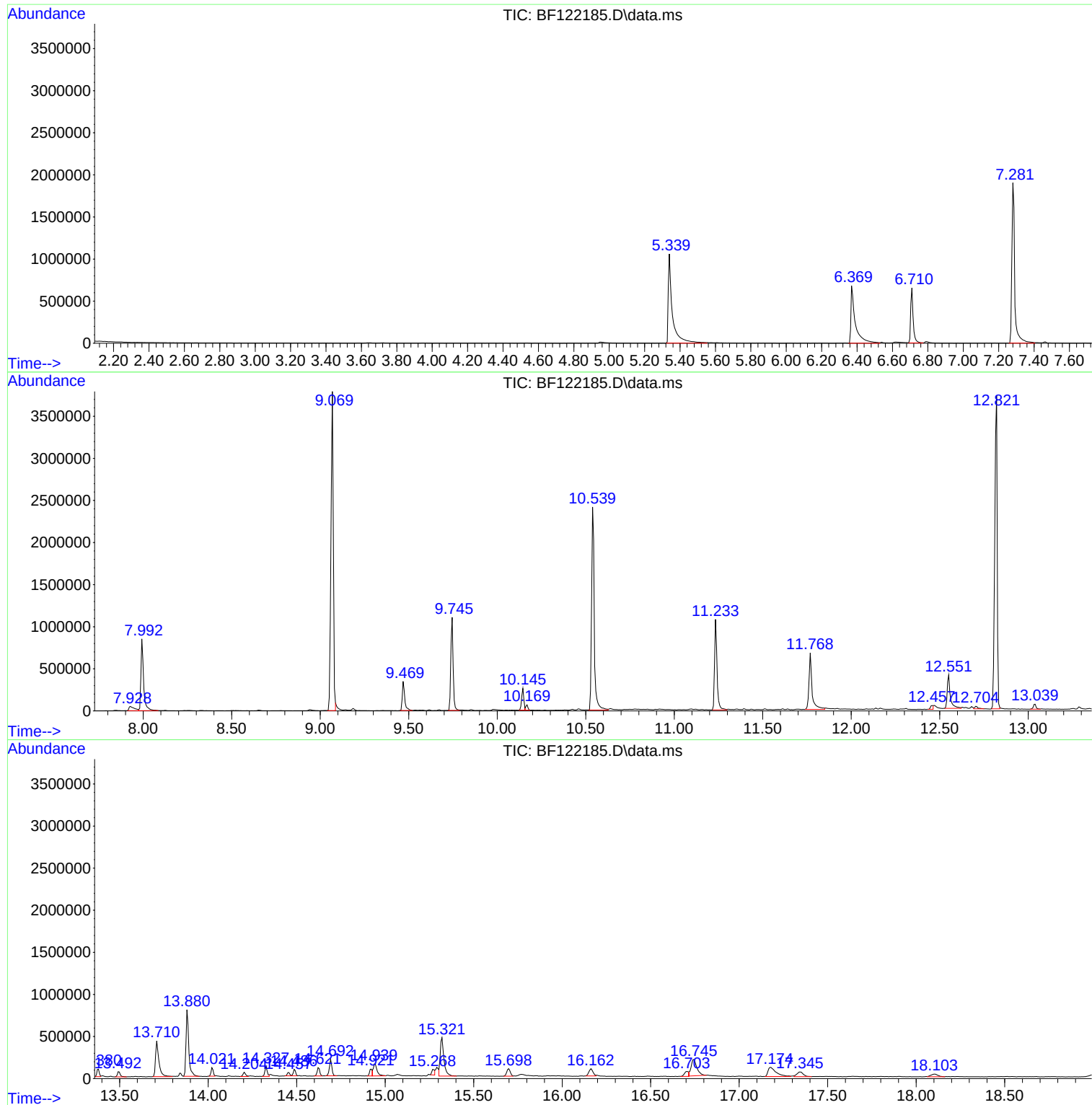
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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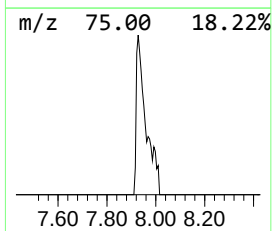
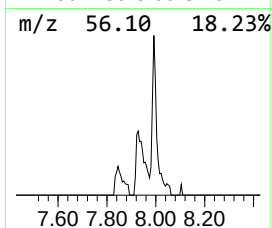
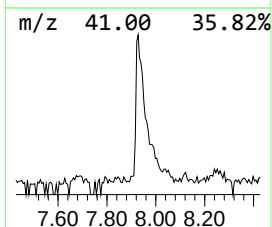
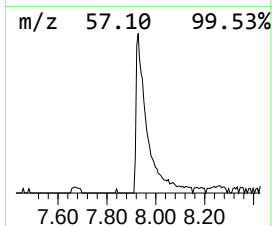
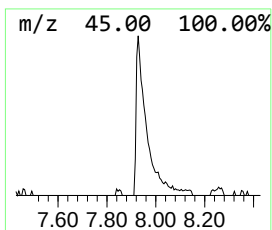
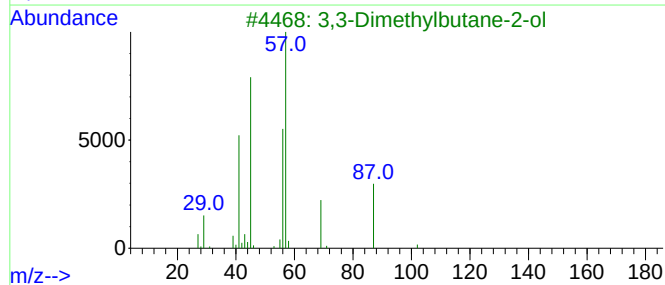
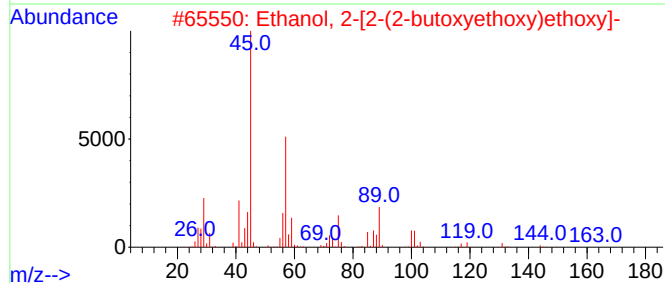
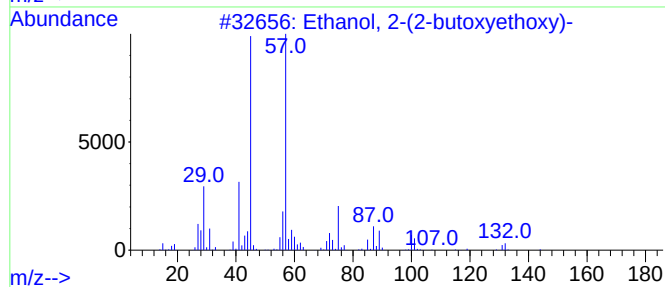
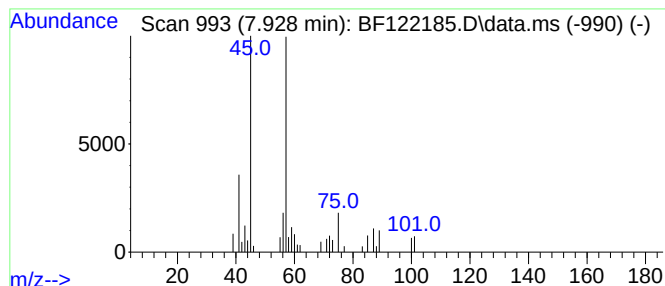
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.928	2.50 ng	108534	Naphthalene-d8	7.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	72
3			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
4			Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	50
5			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	45



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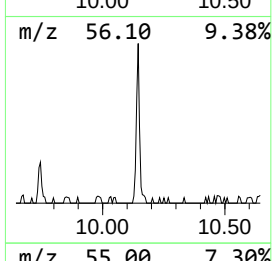
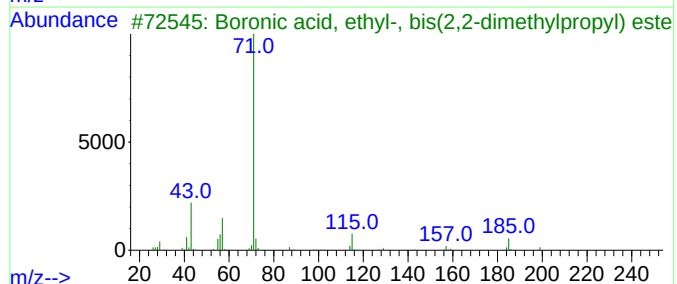
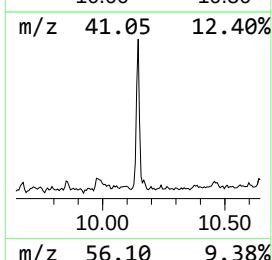
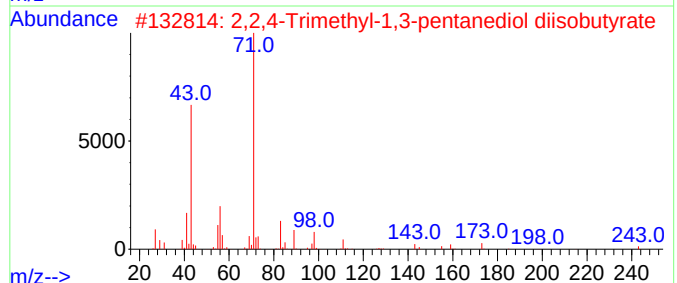
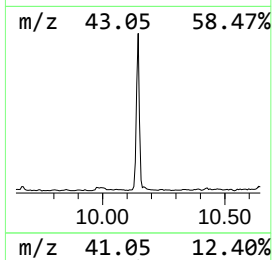
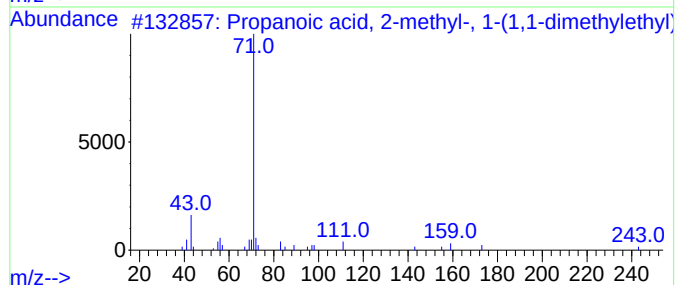
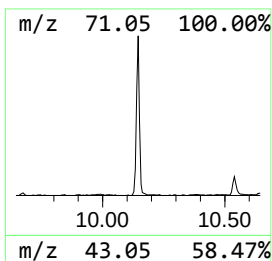
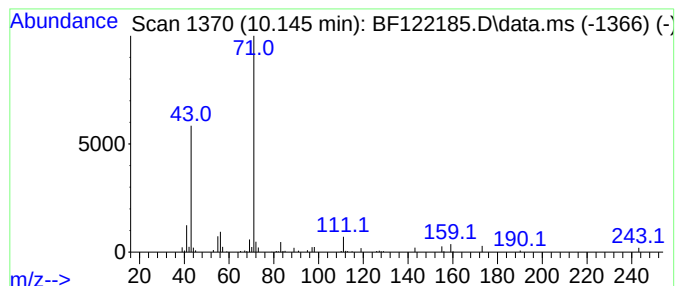
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.145	4.53 ng	220801	Acenaphthene-d10	9.745

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-(1,...	286	C16H30O4	074381-40-1	90
2			2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	78
3			Boronic acid, ethyl-, bis(2,2-di...	214	C12H27B02	067753-47-3	50
4			Butanoic acid, 2-butoxy-1-methyl...	216	C11H20O4	007492-70-8	50
5			Pentanoic acid, 2,2,4-trimethyl-...	286	C16H30O4	1000140-77-5	47



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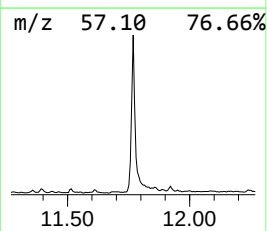
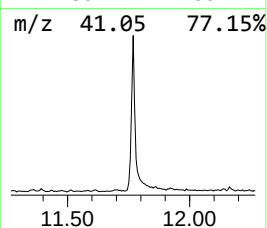
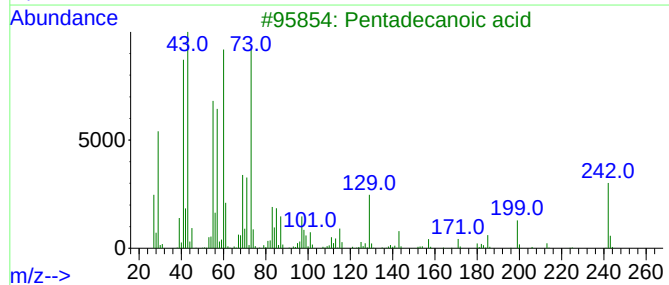
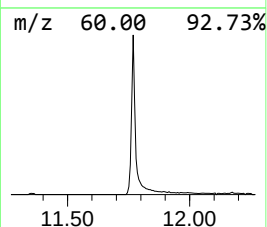
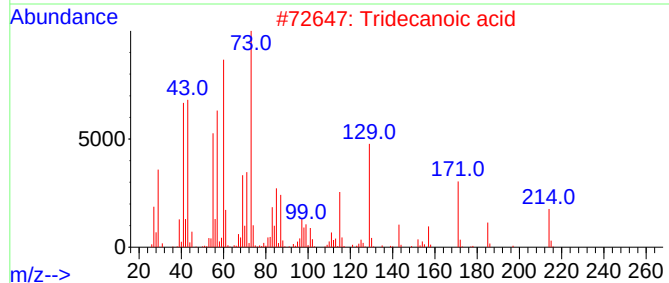
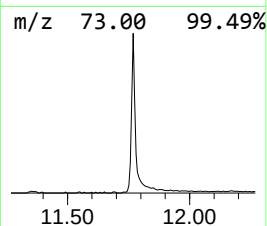
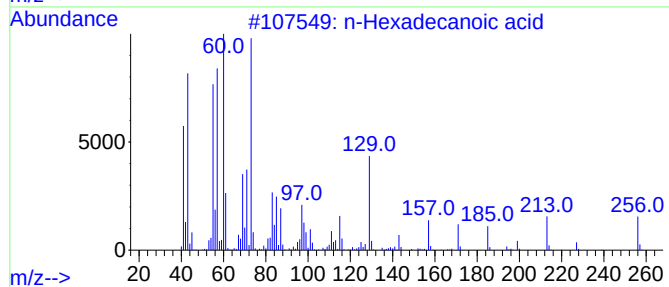
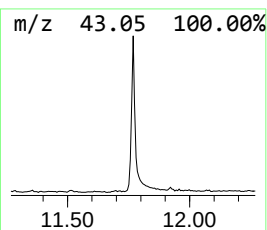
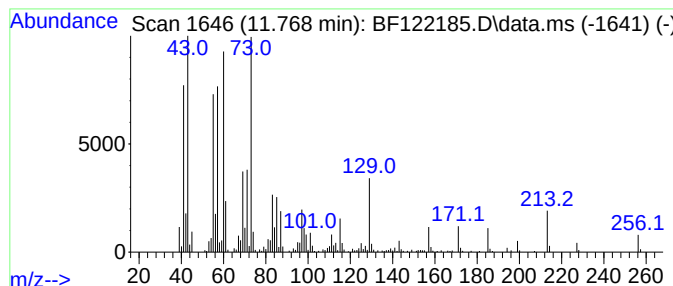
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.769	15.63 ng	805238	Phenanthrene-d10	11.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20



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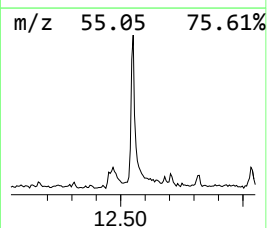
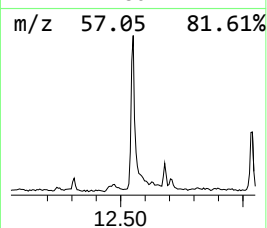
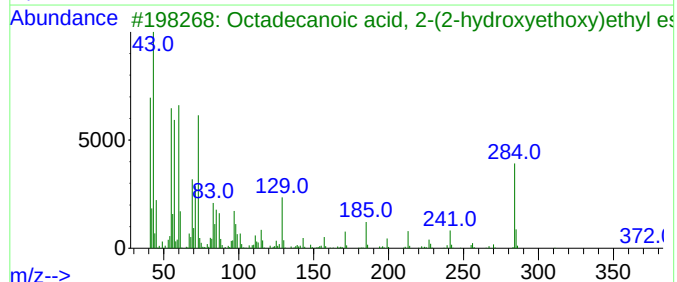
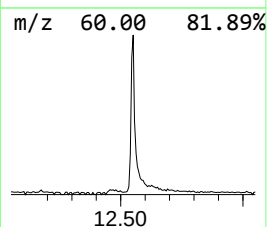
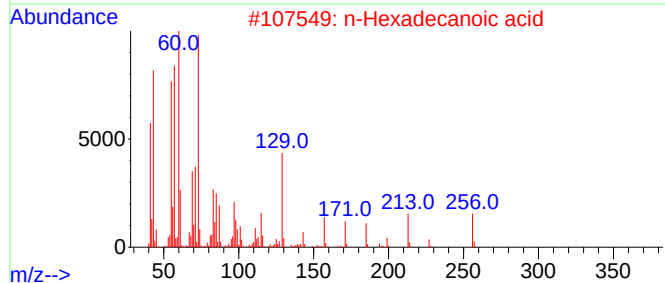
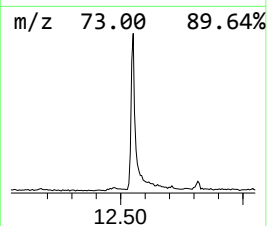
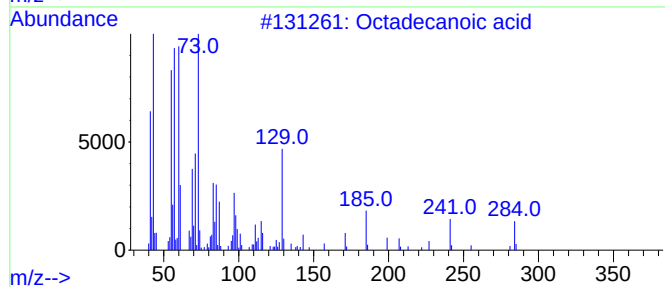
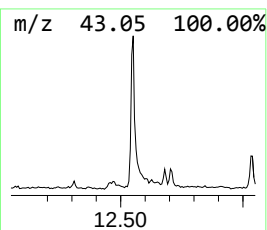
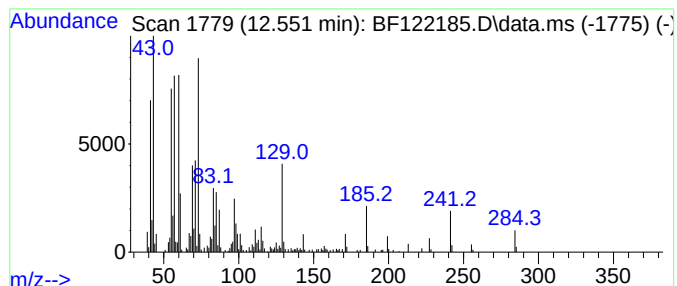
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.551	9.29 ng	478884	Phenanthrene-d10	11.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	83



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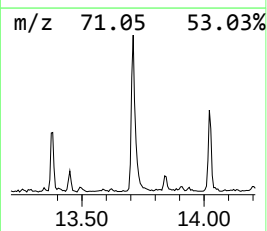
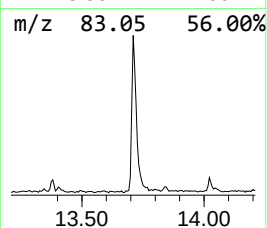
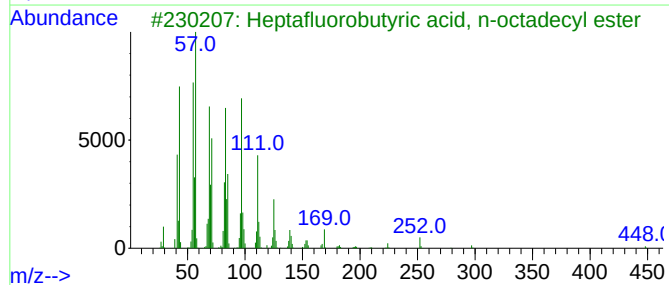
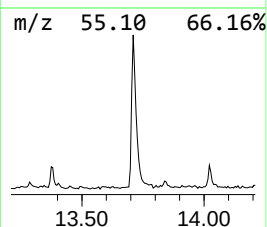
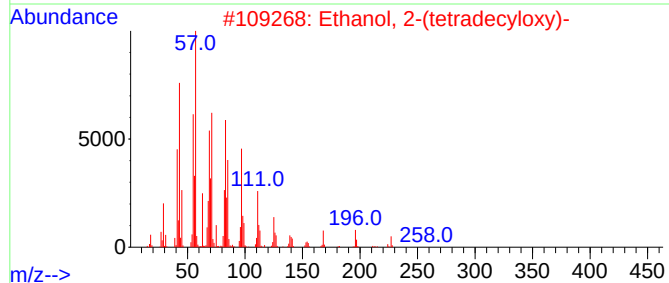
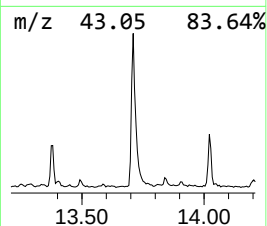
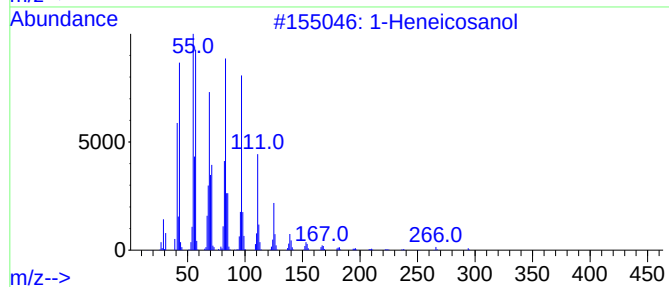
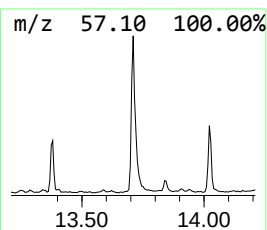
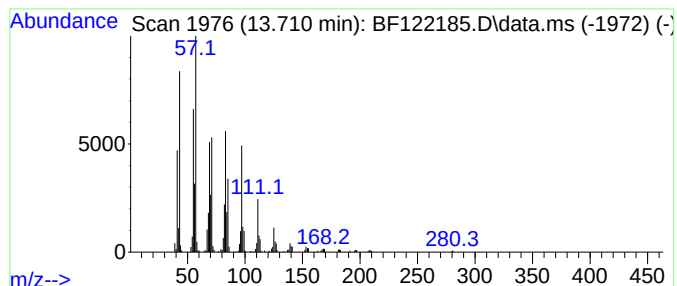
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.710	13.20 ng	561172	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	93
2			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3			Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	91
4			Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
5			1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
Data File : BF122185.D
Acq On : 30 Oct 2020 17:42
Operator : JU/CG
Sample : L4532-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IB1-TREATED-EFFLU

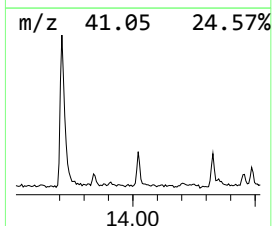
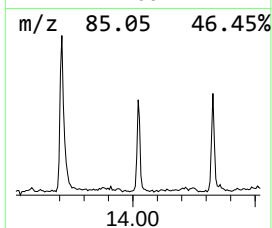
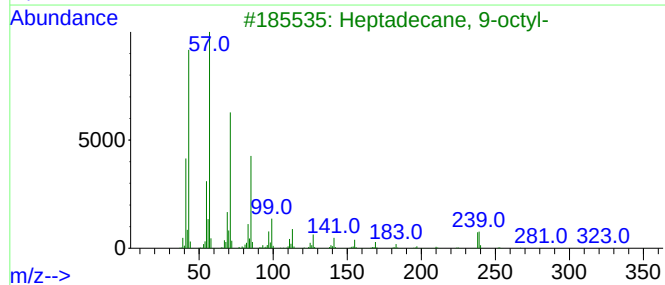
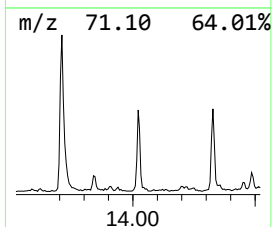
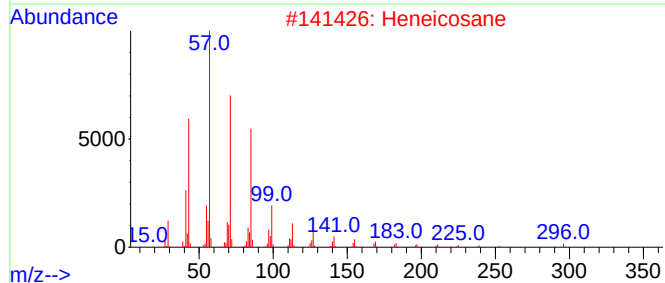
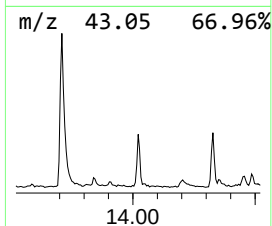
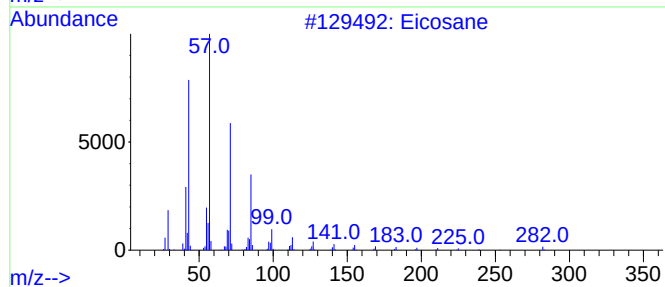
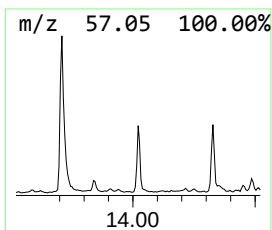
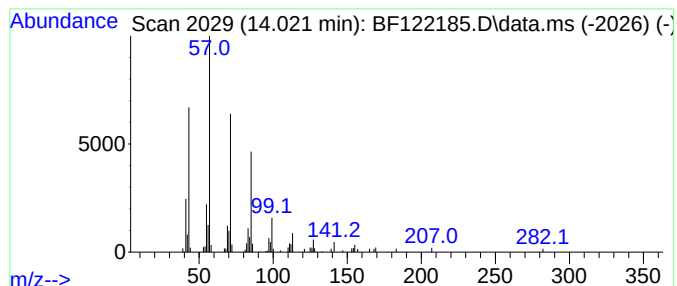
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.021	2.09 ng	88665	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	96
2			Heneicosane	296	C21H44	000629-94-7	91
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4			Heptacosane	380	C27H56	000593-49-7	91
5			Hexadecane	226	C16H34	000544-76-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
Data File : BF122185.D
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Misc :
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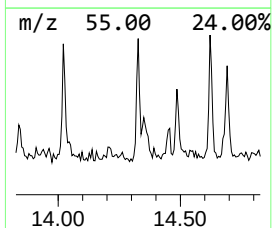
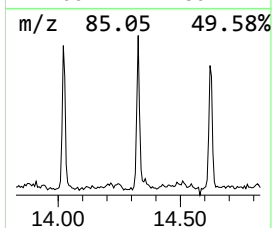
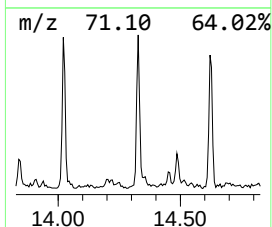
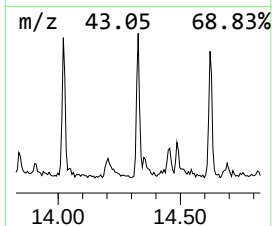
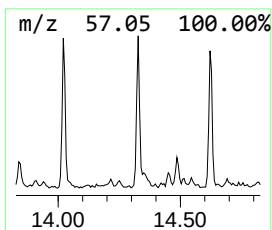
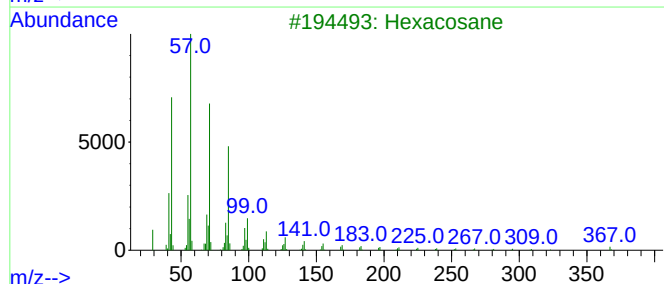
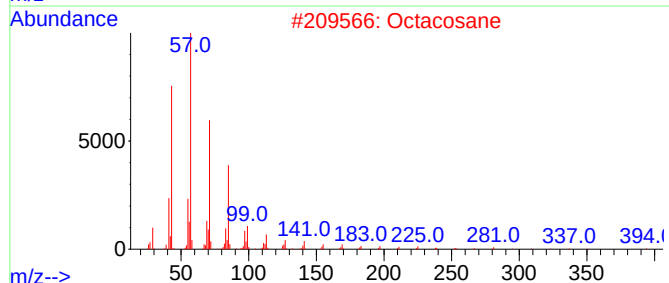
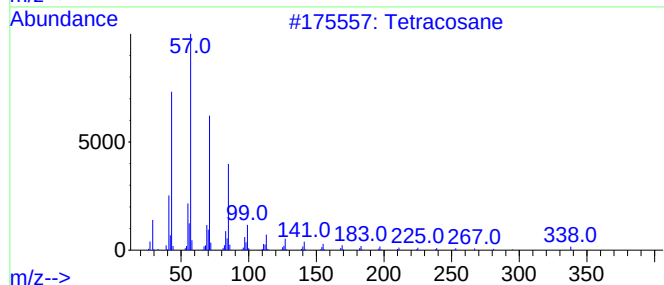
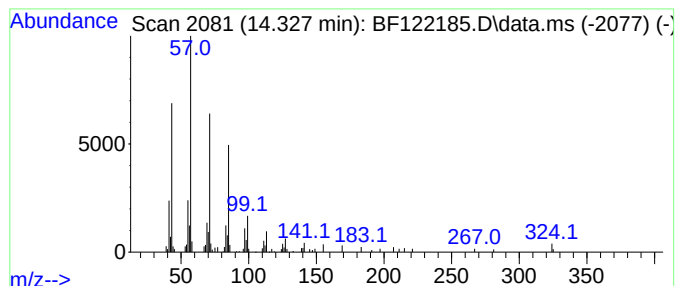
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetracosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.327	2.58 ng	109789	Chrysene-d12	13.880	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	90
2	Octacosane	394	C28H58	000630-02-4	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Eicosane, 2-methyl-	296	C21H44	001560-84-5	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
Data File : BF122185.D
Acq On : 30 Oct 2020 17:42
Operator : JU/CG
Sample : L4532-01
Misc :
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Instrument :
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ClientSampleId :
IB1-TREATED-EFFLU

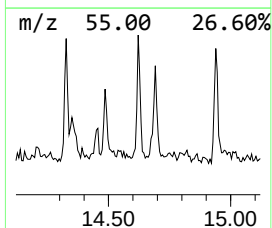
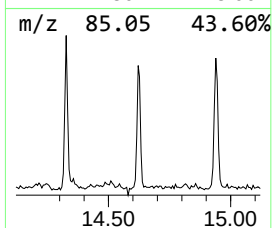
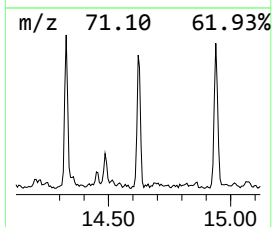
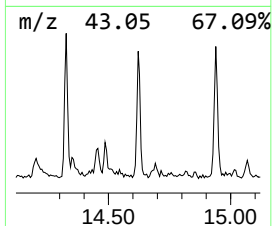
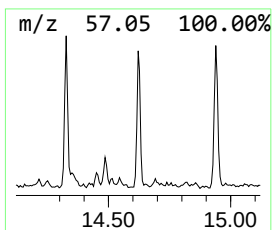
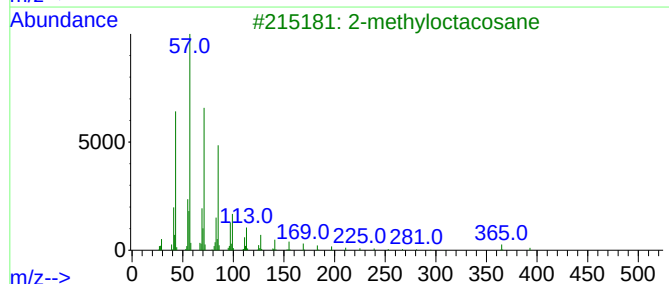
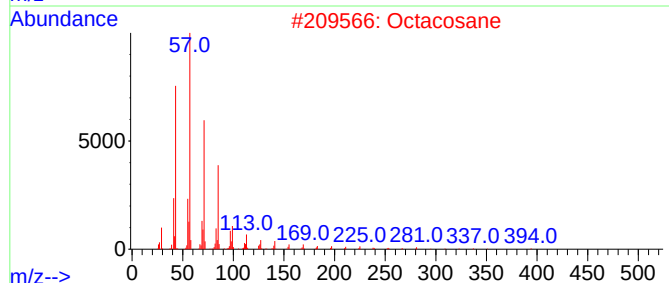
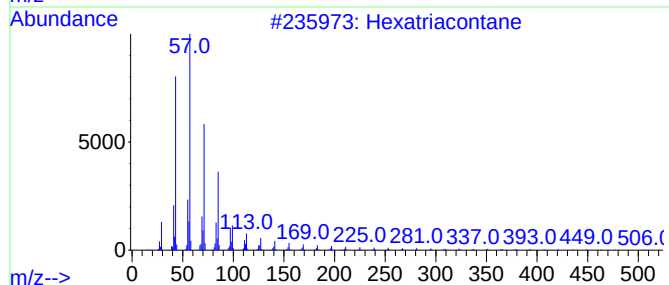
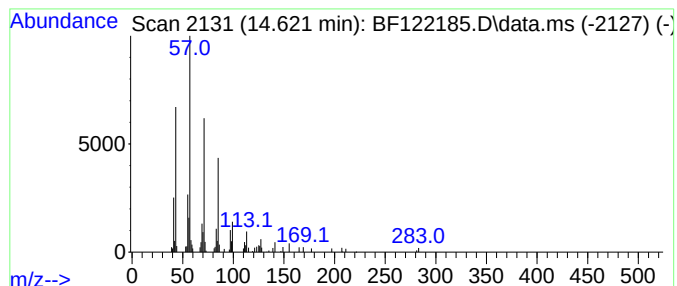
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexatriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.621	2.99 ng	97070	Perylene-d12	15.321

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexatriacontane	507	C36H74	000630-06-8	91
2			Octacosane	394	C28H58	000630-02-4	91
3			2-methyloctacosane	408	C29H60	1000376-72-8	91
4			Hexacosane	366	C26H54	000630-01-3	91
5			Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
Data File : BF122185.D
Acq On : 30 Oct 2020 17:42
Operator : JU/CG
Sample : L4532-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IB1-TREATED-EFFLU

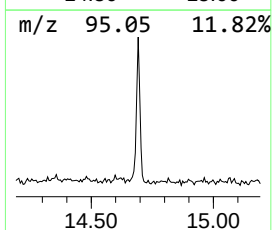
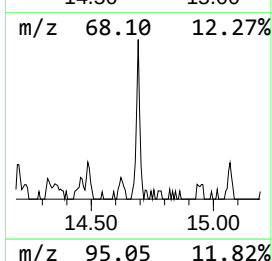
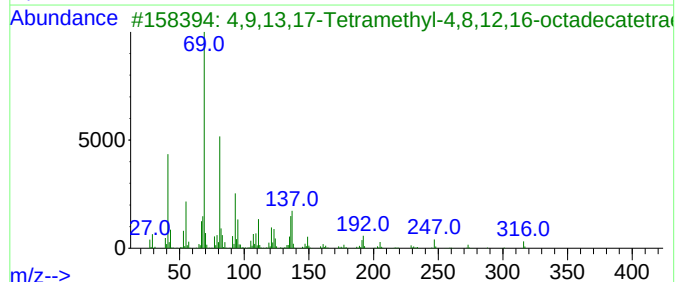
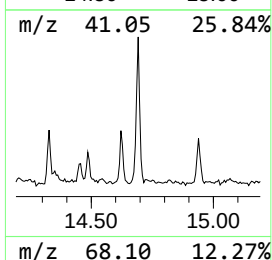
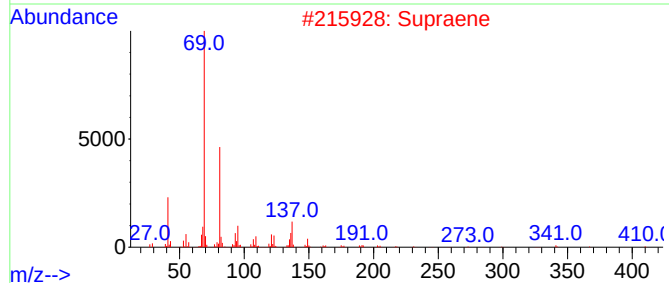
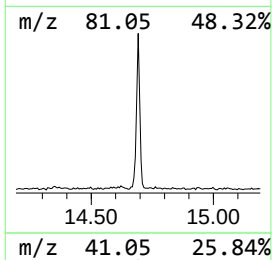
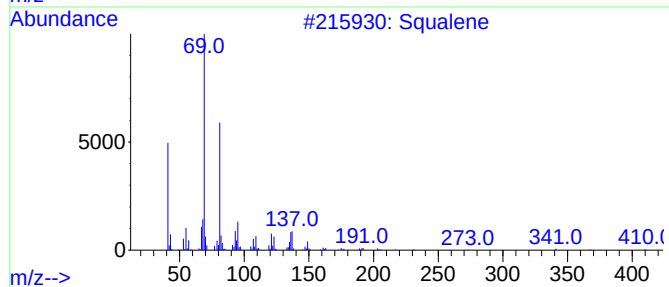
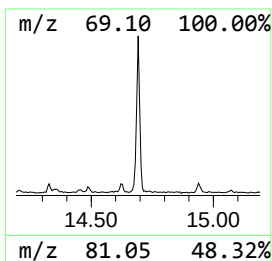
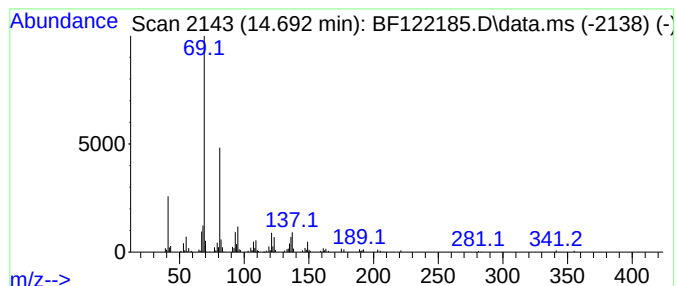
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.692	5.86 ng	190406	Perylene-d12	15.321

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	91
2			Supraene	410	C30H50	007683-64-9	90
3			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
5			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
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Operator : JU/CG
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Misc :
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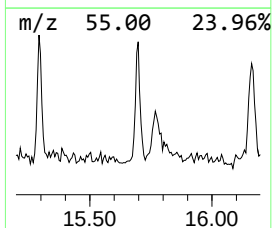
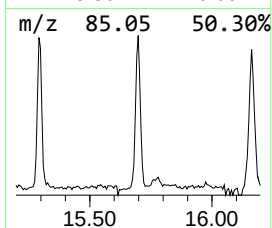
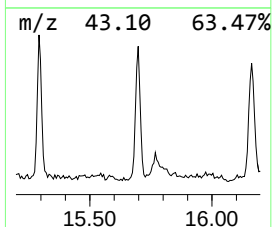
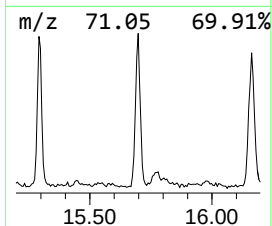
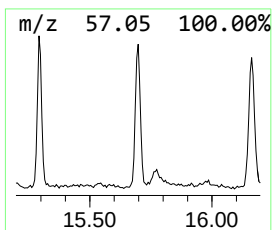
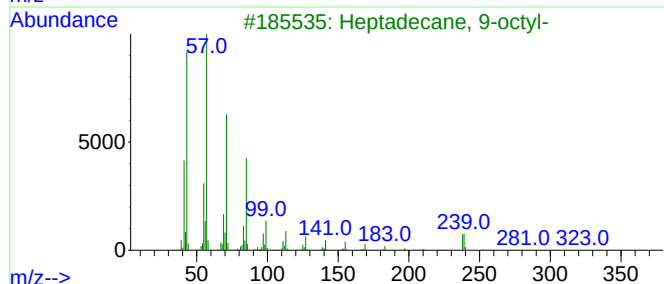
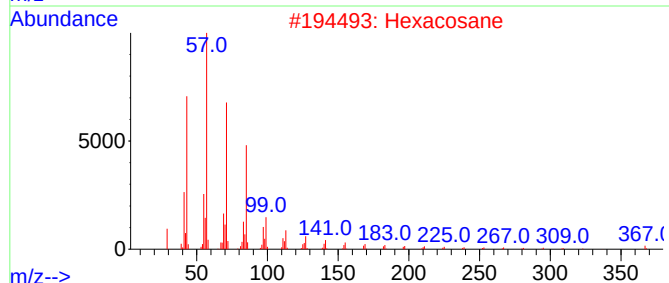
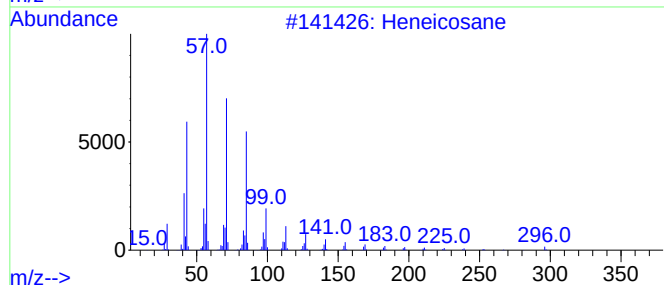
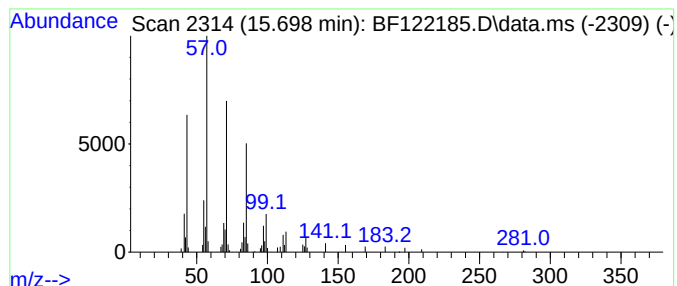
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.698	3.89 ng	126515	Perylene-d12	15.321

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4			Heptadecane	240	C17H36	000629-78-7	87
5			Tetracosane	338	C24H50	000646-31-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
Data File : BF122185.D
Acq On : 30 Oct 2020 17:42
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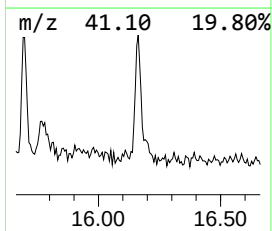
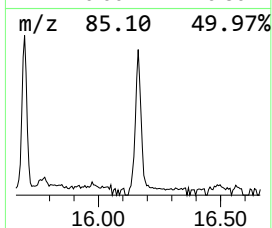
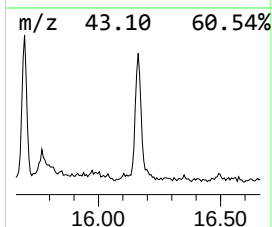
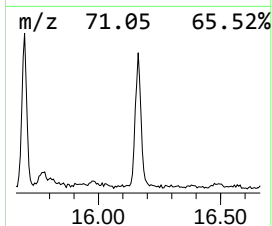
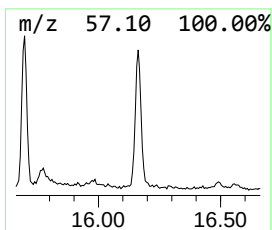
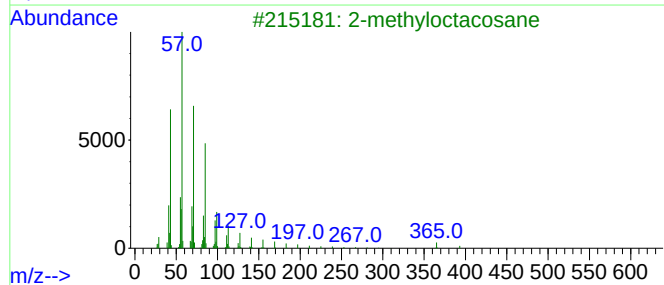
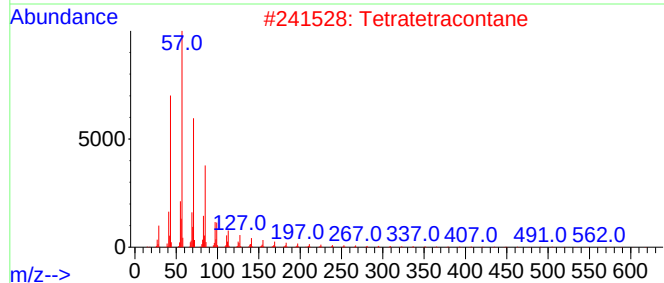
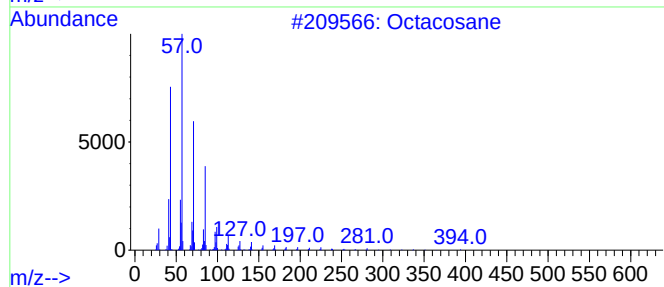
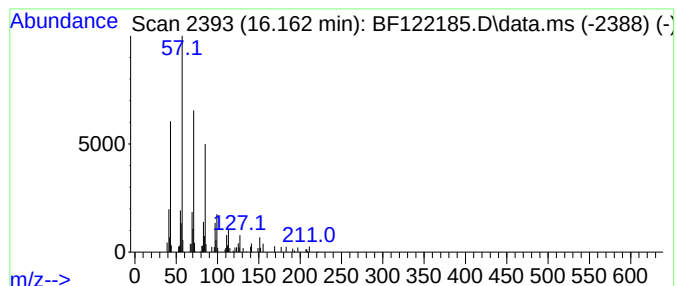
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.162	4.24 ng	137715	Perylene-d12	15.321

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Tetratetracontane	619	C44H90	007098-22-8	91
3			2-methyloctacosane	408	C29H60	1000376-72-8	91
4			Heneicosane	296	C21H44	000629-94-7	91
5			Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
Data File : BF122185.D
Acq On : 30 Oct 2020 17:42
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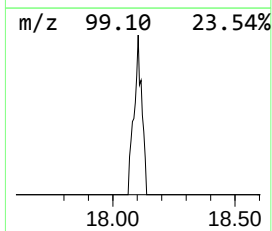
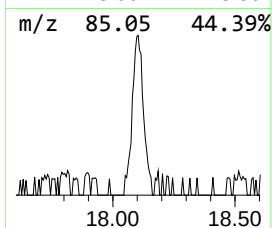
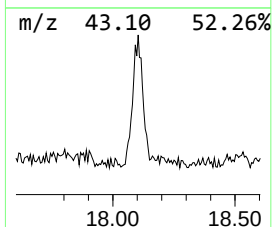
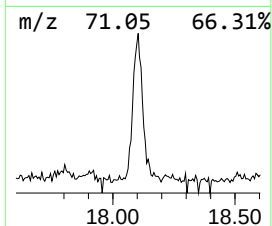
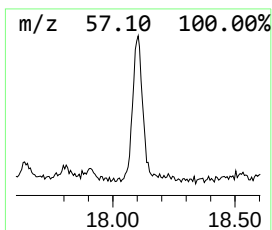
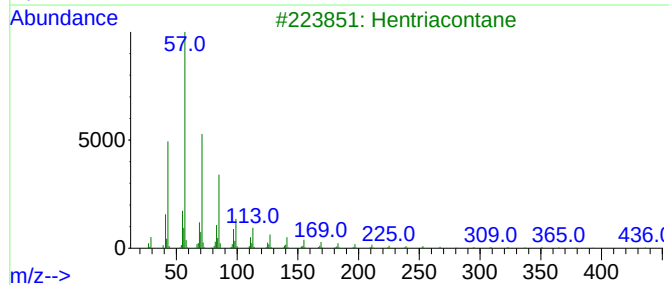
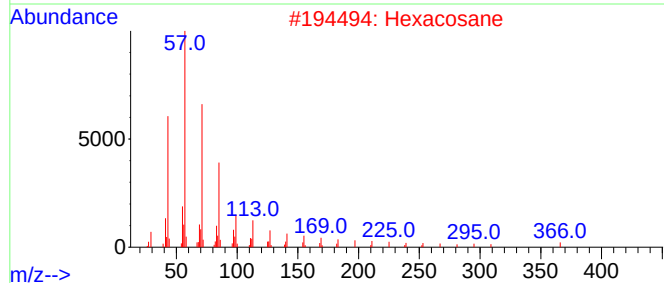
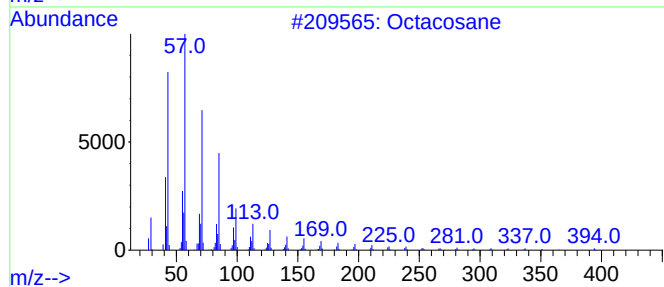
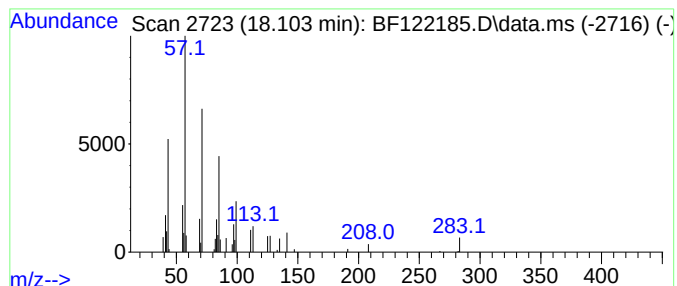
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.103	2.59 ng	84017	Perylene-d12	15.321

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	86
2			Hexacosane	366	C26H54	000630-01-3	80
3			Hentriacontane	437	C31H64	000630-04-6	80
4			Pentacosane	352	C25H52	000629-99-2	80
5			10-Methylnonadecane	282	C20H42	056862-62-5	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
Data File : BF122185.D
Acq On : 30 Oct 2020 17:42
Operator : JU/CG
Sample : L4532-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IB1-TREATED-EFFLU

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-(2-b...	7.928	2.5	ng	108534	2	7.992	868508	20.0
Propanoic acid,...	10.145	4.5	ng	220801	3	9.745	975881	20.0
n-Hexadecanoic ...	11.769	15.6	ng	805238	4	11.233	1030610	20.0
Octadecanoic acid	12.551	9.3	ng	478884	4	11.233	1030610	20.0
1-Heneicosanol	13.710	13.2	ng	561172	5	13.880	849981	20.0
Eicosane	14.021	2.1	ng	88665	5	13.880	849981	20.0
Tetracosane	14.327	2.6	ng	109789	5	13.880	849981	20.0
Hexatriacontane	14.621	3.0	ng	97070	6	15.321	649693	20.0
Squalene	14.692	5.9	ng	190406	6	15.321	649693	20.0
Heneicosane	15.698	3.9	ng	126515	6	15.321	649693	20.0
Octacosane	16.162	4.2	ng	137715	6	15.321	649693	20.0
Triacontane	17.345	4.2	ng	135954	6	15.321	649693	20.0
Hexacosane	18.103	2.6	ng	84017	6	15.321	649693	20.0