

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP032822\
 Data File : BP009577.D
 Acq On : 28 Mar 2022 21:43
 Operator : CG/JU
 Sample : N2103-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 CHRT-2001

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_P\Methods\8270E-BP031722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP009577.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.023	3	6	27	rVB	790491	1208479	8.02%	1.067%
2	5.375	399	406	428	rBV	3516526	6309785	41.87%	5.571%
3	6.958	663	675	695	rBV	3268977	6526472	43.31%	5.763%
4	7.763	804	812	829	rBV	885662	1698351	11.27%	1.500%
5	8.922	1002	1009	1020	rBV	2243146	4096755	27.19%	3.617%
6	9.163	1044	1050	1067	rVB	59746	164700	1.09%	0.145%
7	10.557	1277	1287	1293	rBV	1189727	2252667	14.95%	1.989%
8	10.604	1293	1295	1304	rVB	102172	186389	1.24%	0.165%
9	13.028	1700	1707	1729	rBV	6229360	10642876	70.62%	9.398%
10	14.134	1889	1895	1907	rBV	433367	752344	4.99%	0.664%
11	14.410	1933	1942	1949	rBV	1994822	3203891	21.26%	2.829%
12	14.475	1949	1953	1963	rVB	126598	247001	1.64%	0.218%
13	15.022	2041	2046	2051	rBV3	87950	198926	1.32%	0.176%
14	15.287	2086	2091	2097	rBV2	129106	213168	1.41%	0.188%
15	15.463	2117	2121	2133	rVB3	108912	298140	1.98%	0.263%
16	15.910	2190	2197	2206	rBV	5069821	8153286	54.10%	7.199%
17	16.151	2234	2238	2240	rBV4	118217	182646	1.21%	0.161%
18	17.175	2406	2412	2416	rBV	2375688	3666950	24.33%	3.238%
19	17.216	2416	2419	2427	rVV	763395	1159562	7.69%	1.024%
20	17.310	2430	2435	2441	rVB	419680	654979	4.35%	0.578%
21	18.051	2558	2561	2563	rBV	141962	165904	1.10%	0.146%
22	18.086	2563	2567	2575	rVB2	574546	964925	6.40%	0.852%
23	18.239	2588	2593	2597	rBV2	400595	719589	4.78%	0.635%
24	18.951	2710	2714	2718	rBV	281269	414101	2.75%	0.366%
25	19.157	2746	2749	2752	rVB2	275424	304259	2.02%	0.269%
26	19.204	2752	2757	2762	rVB	2127041	2771434	18.39%	2.447%
27	19.351	2779	2782	2787	rVB	287463	360846	2.39%	0.319%
28	19.557	2809	2817	2826	rVB	2561467	4240241	28.14%	3.744%
29	19.757	2845	2851	2856	rBV	11789252	15069741	100.00%	13.306%
30	19.875	2868	2871	2879	rVB3	321640	586419	3.89%	0.518%
31	20.139	2913	2916	2919	rBV2	334772	397733	2.64%	0.351%
32	20.198	2924	2926	2930	rVB	353394	372730	2.47%	0.329%
33	20.333	2947	2949	2953	rVB	280685	308598	2.05%	0.272%
34	21.027	3063	3067	3082	rVB5	1060523	2768028	18.37%	2.444%
35	21.216	3094	3099	3104	rVB	9643656	11791086	78.24%	10.411%
36	21.292	3106	3112	3116	rVV3	3672949	6676951	44.31%	5.896%

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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_P\Methods\8270E-BP031722.M
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37	21.327	3116	3118	3128	rVB	1375597	1854633	12.31%	1.638%
38	21.410	3129	3132	3136	rBV	664911	903881	6.00%	0.798%
39	22.963	3391	3396	3402	rBV	1169874	2775184	18.42%	2.450%
40	23.474	3480	3483	3493	rVB	831767	1569356	10.41%	1.386%
41	23.580	3496	3501	3509	rVB	1284771	2662062	17.66%	2.351%
42	23.686	3513	3519	3525	rBV2	1806655	3756502	24.93%	3.317%

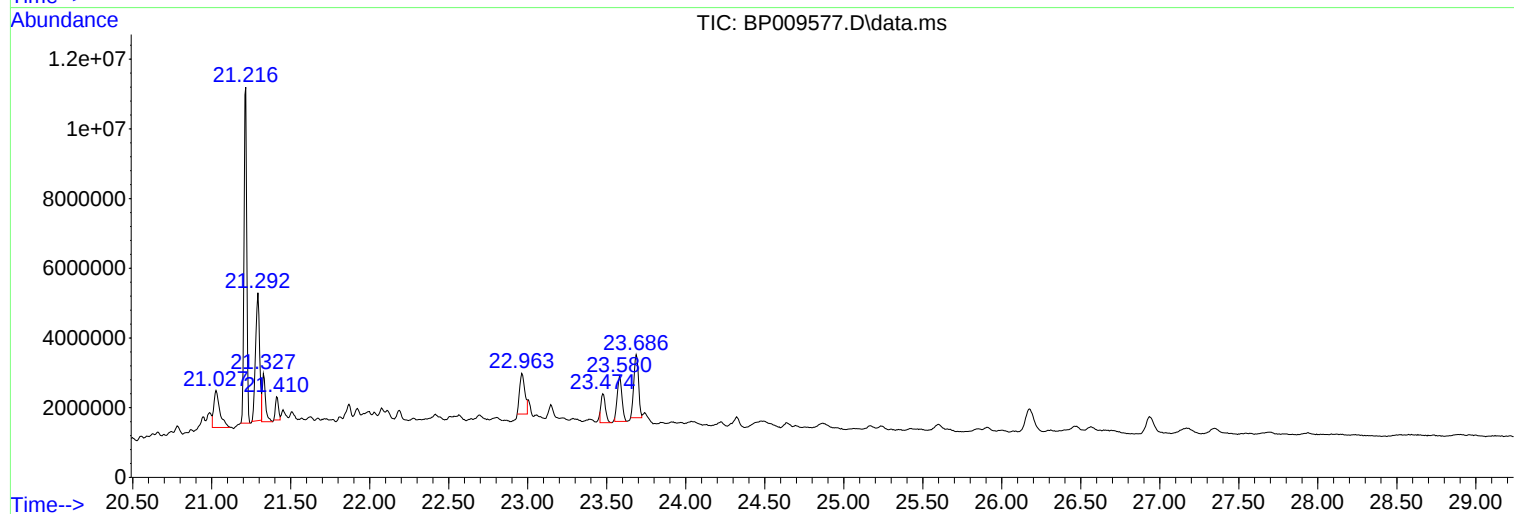
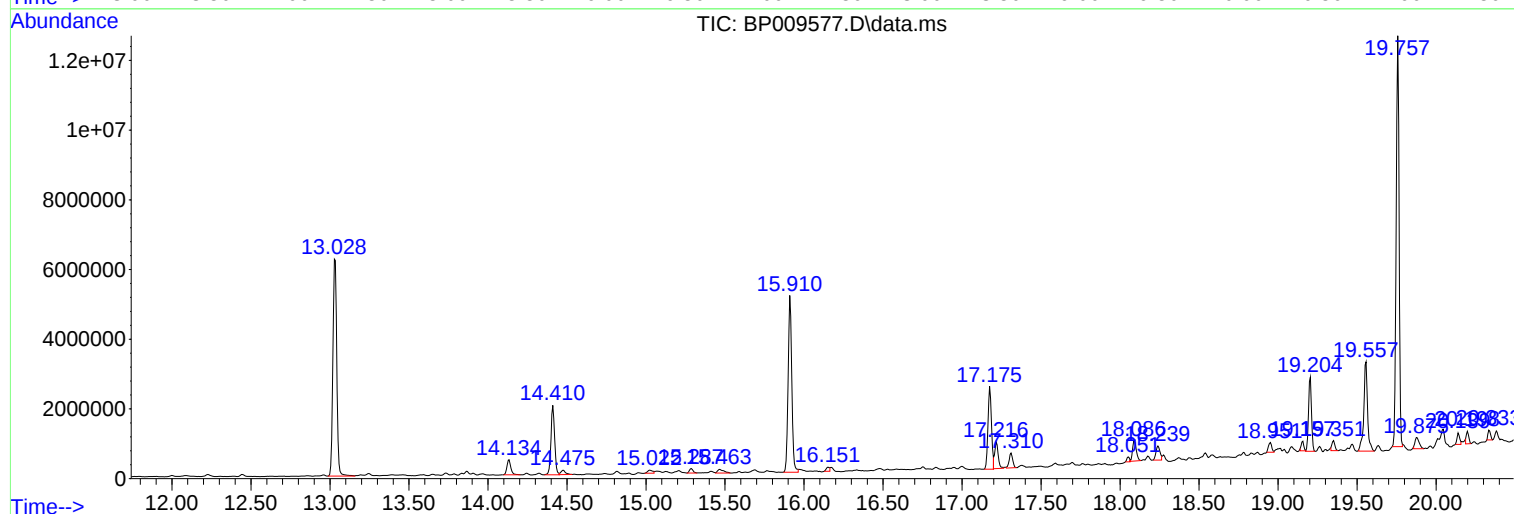
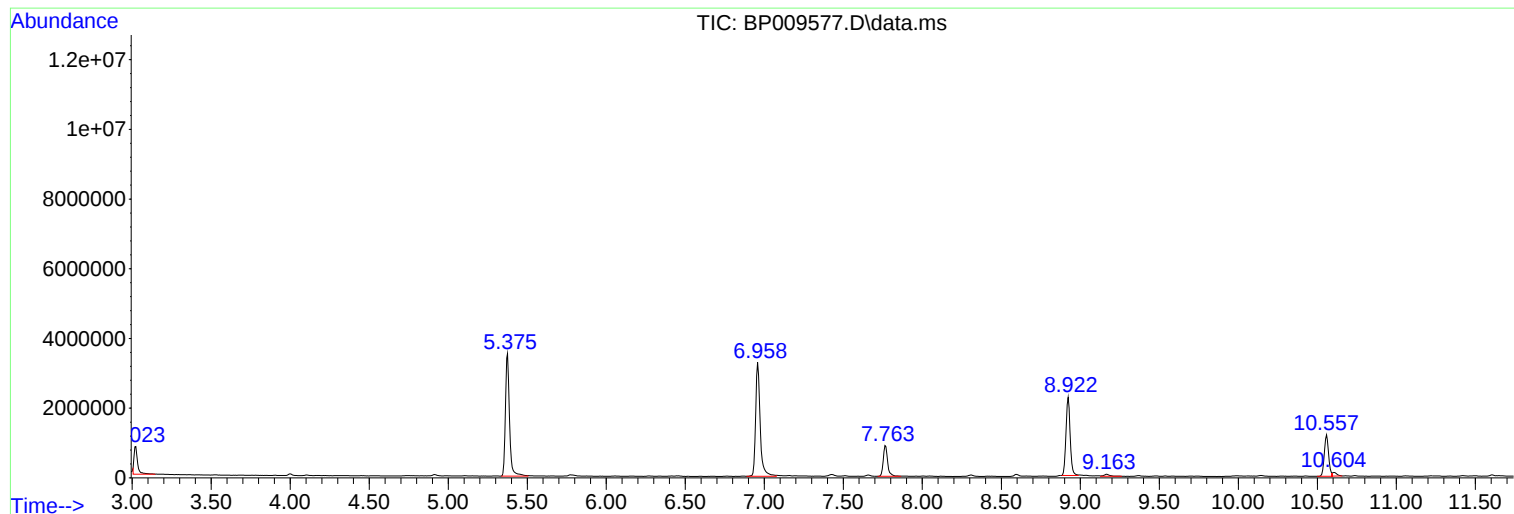
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BP009577.D
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Operator : CG/JU
Sample : N2103-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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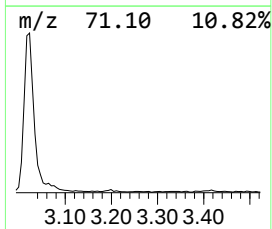
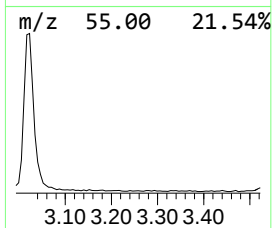
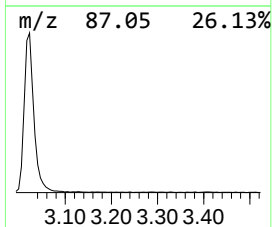
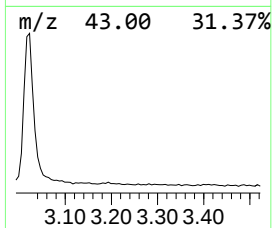
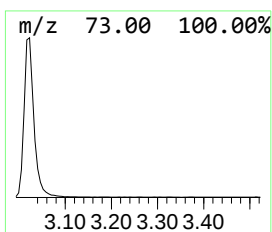
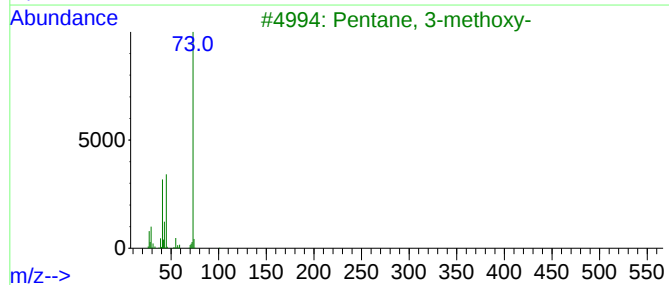
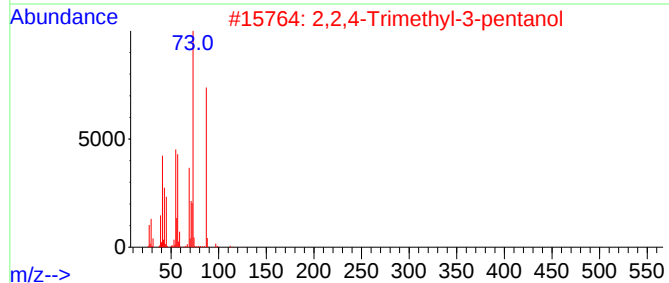
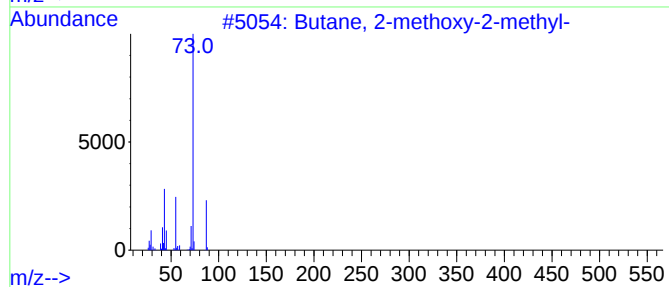
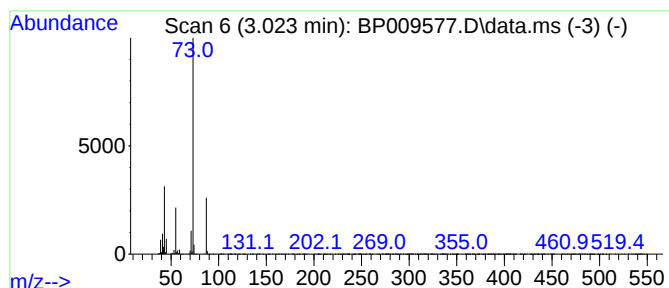
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.023	14.23 ng	1208480	1,4-Dichlorobenzene-d4	7.763

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	43
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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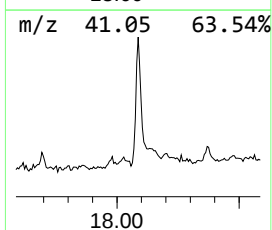
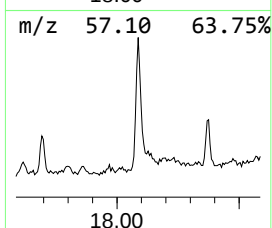
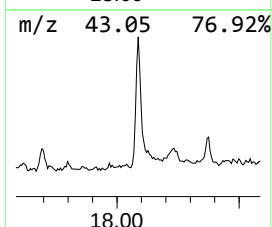
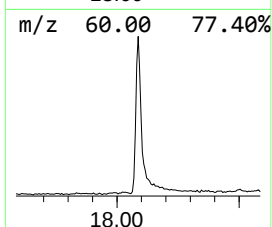
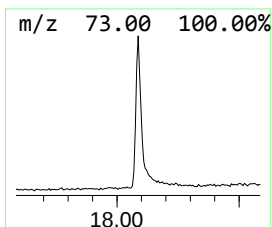
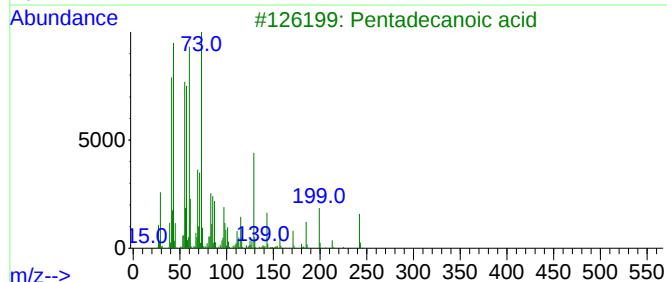
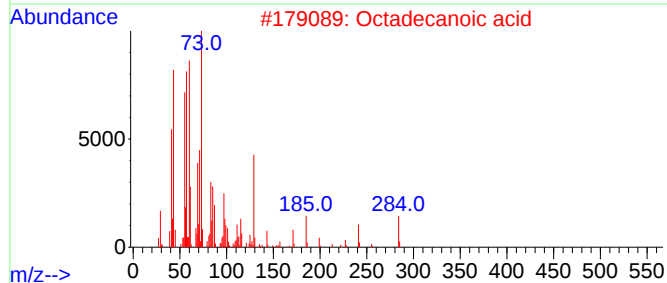
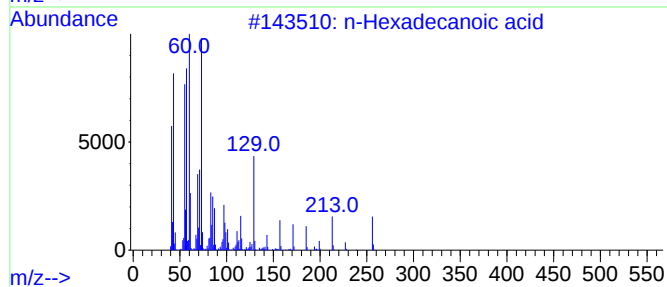
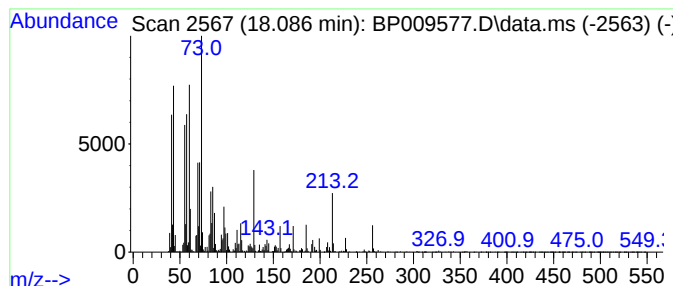
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.086	5.26 ng	964925	Phenanthrene-d10	17.175

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Octadecanoic acid	284	C18H36O2	000057-11-4	87
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4		n-Decanoic acid	172	C10H20O2	000334-48-5	70
5		Tridecanoic acid	214	C13H26O2	000638-53-9	68



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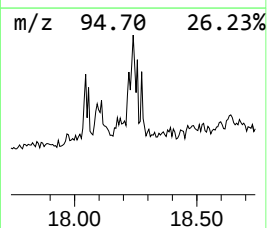
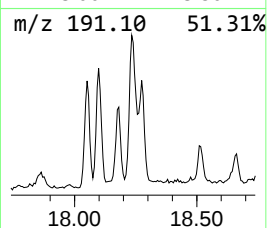
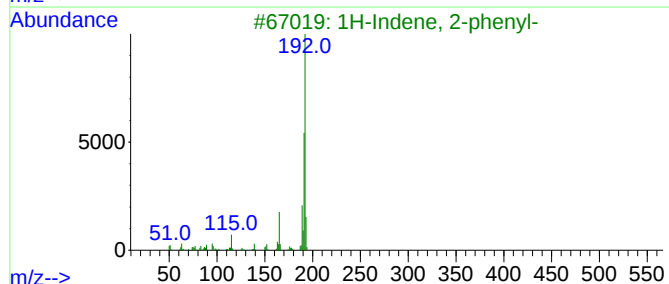
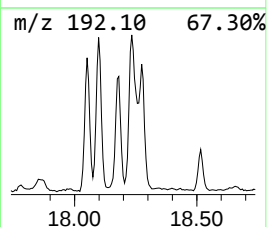
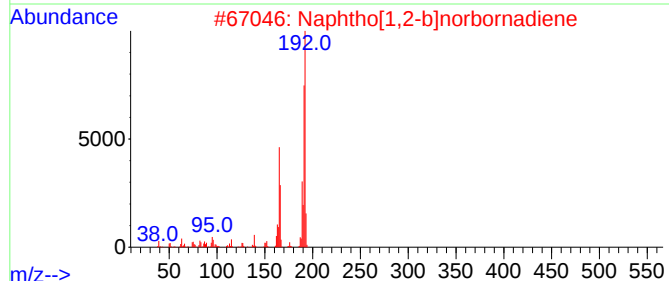
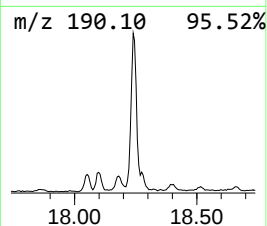
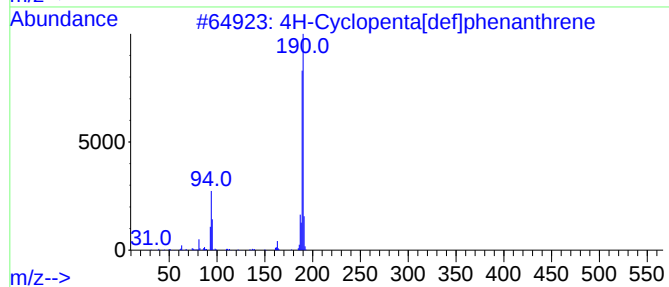
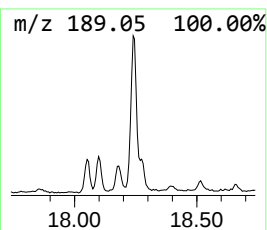
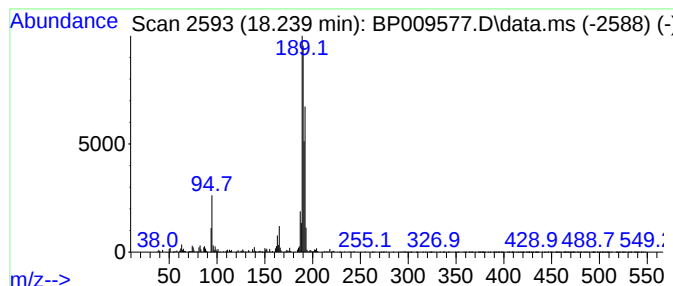
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.239	3.92 ng	719589	Phenanthrene-d10	17.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
2			Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	42
3			1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	38
4			Benzene, 1,1'-(1,2-propadienylid...	192	C15H12	014251-57-1	38
5			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	38



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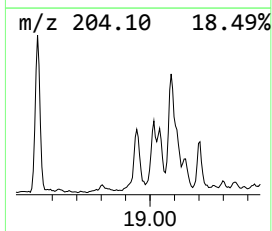
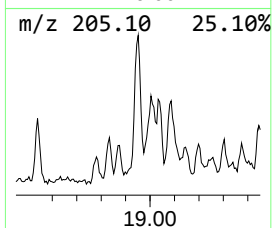
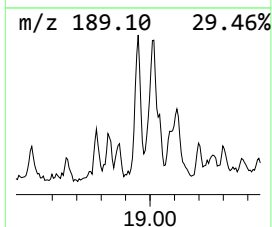
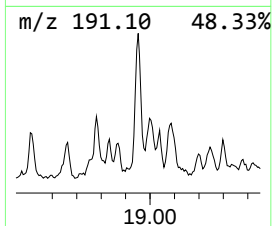
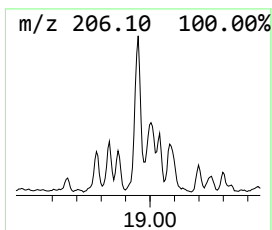
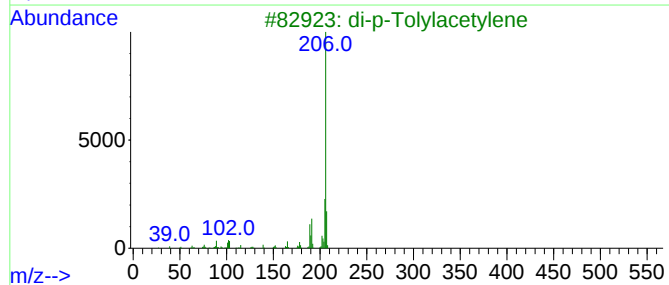
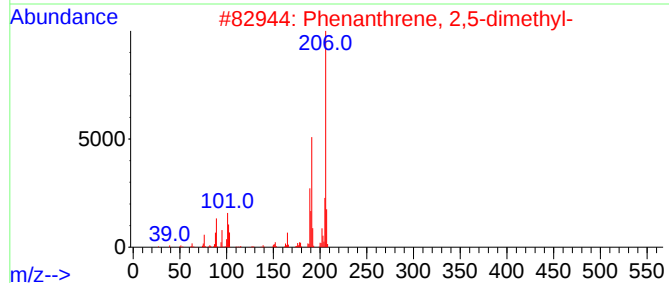
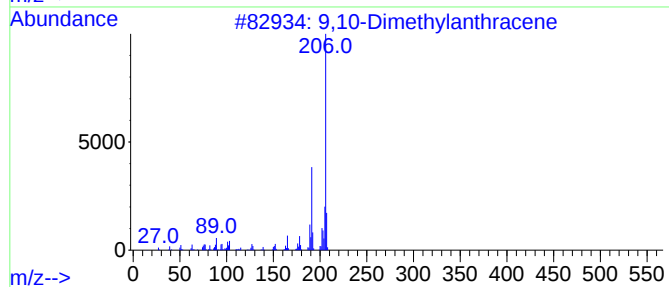
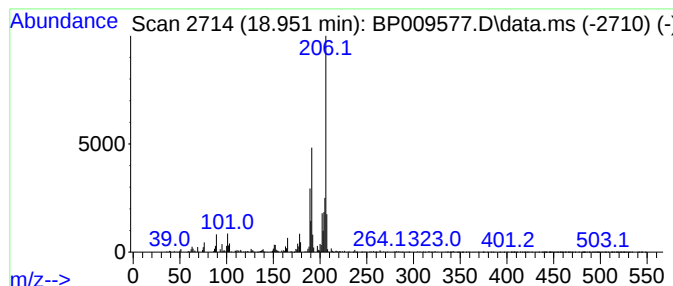
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9,10-Dimethylantracene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.951	2.26 ng	414101	Phenanthrene-d10	17.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,10-Dimethylantracene	206	C16H14	000781-43-1	95
2			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	93
3			di-p-Tolylacetylene	206	C16H14	002789-88-0	91
4			Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	90
5			Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	87



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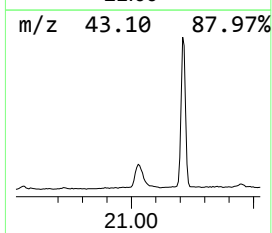
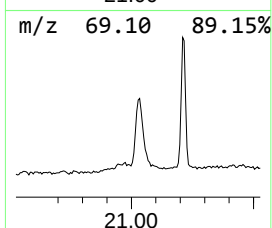
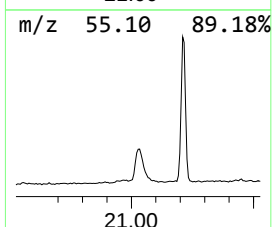
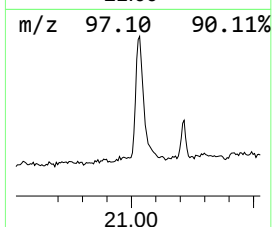
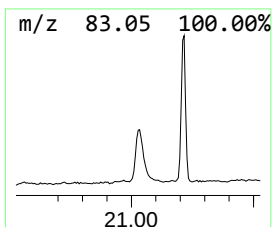
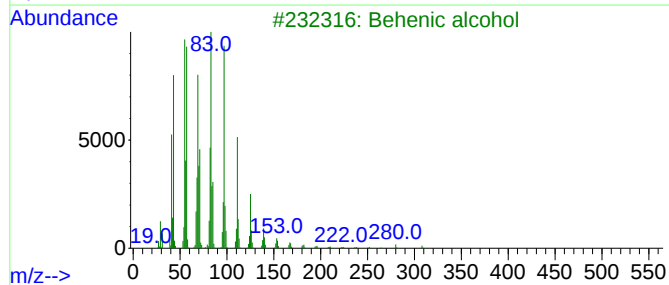
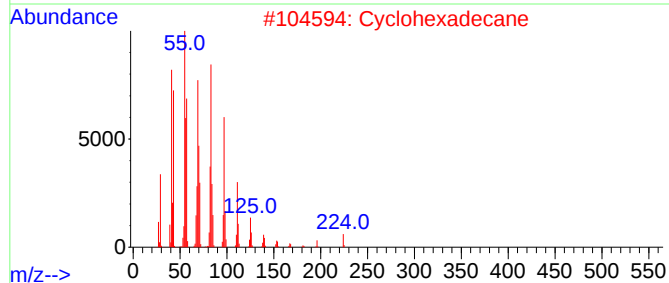
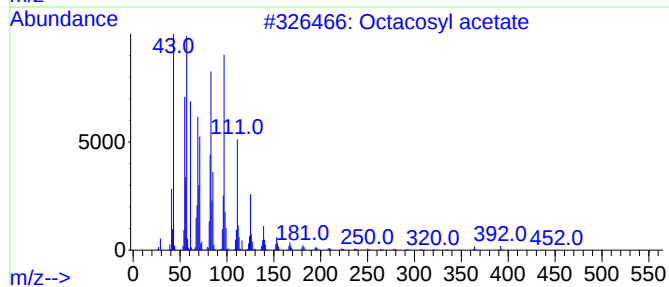
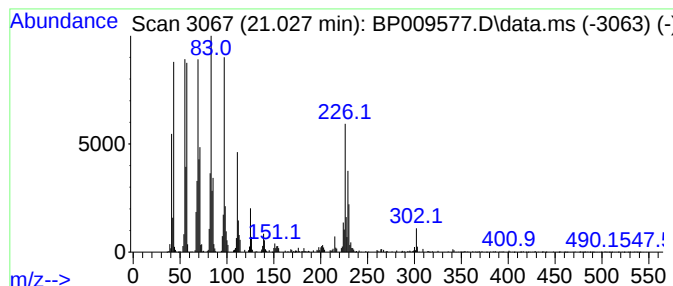
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octacosyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.028	8.29 ng	2768030	Chrysene-d12	21.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosyl acetate	452	C30H60O2	018206-97-8	95
2			Cyclohexadecane	224	C16H32	000295-65-8	94
3			Behenic alcohol	326	C22H46O	000661-19-8	93
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	89
5			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP032822\
Data File : BP009577.D
Acq On : 28 Mar 2022 21:43
Operator : CG/JU
Sample : N2103-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CHRT-2001

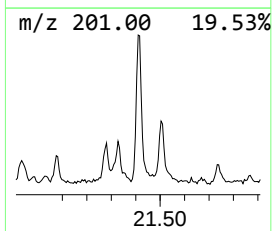
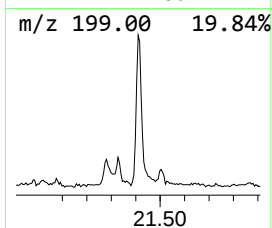
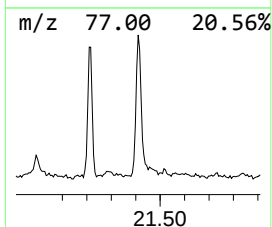
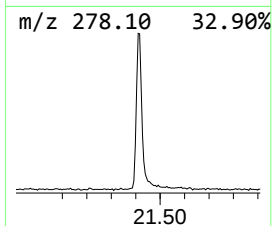
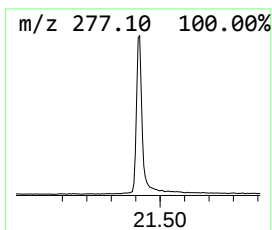
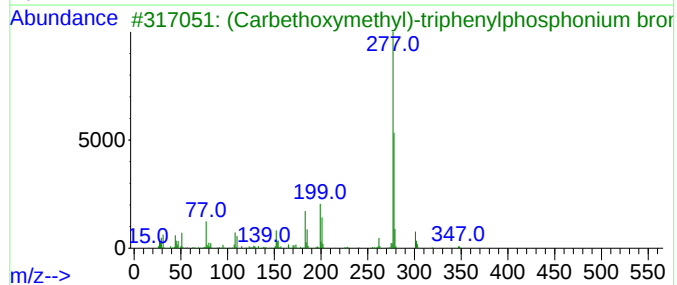
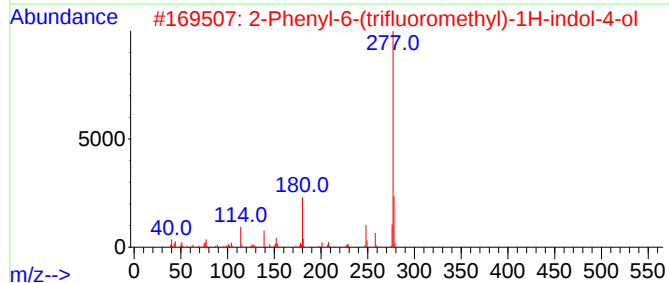
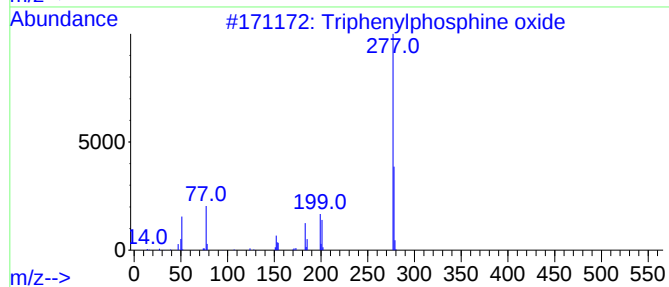
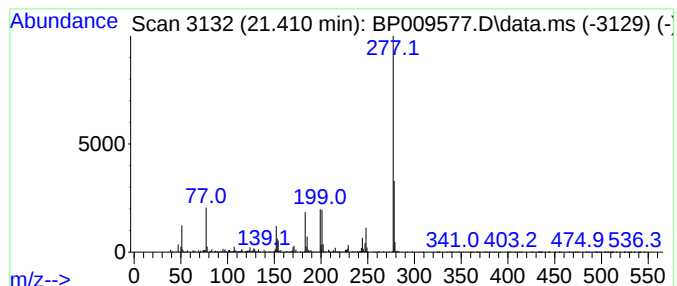
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.410	2.71 ng	903881	Chrysene-d12	21.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	43
3			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	42
4			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	42
5			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19N03S	1000483-83-4	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP032822\
Data File : BP009577.D
Acq On : 28 Mar 2022 21:43
Operator : CG/JU
Sample : N2103-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CHRT-2001

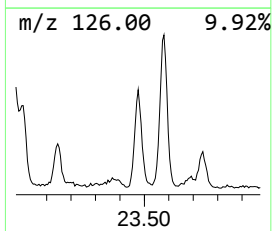
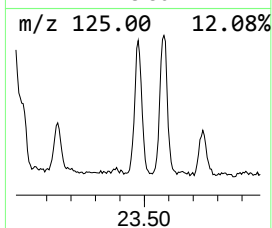
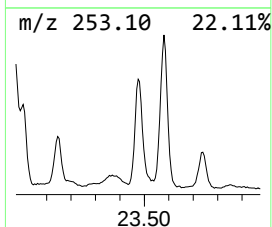
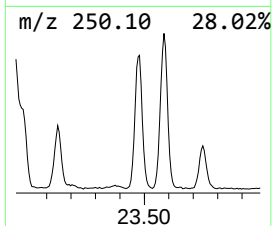
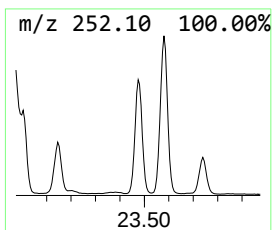
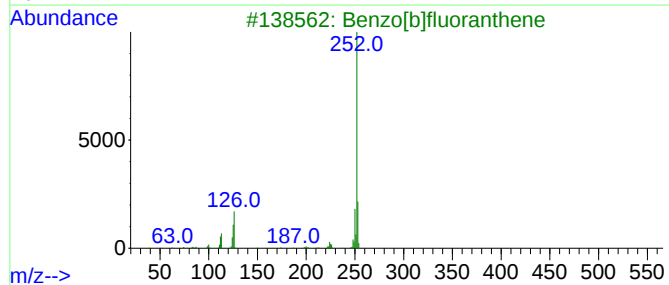
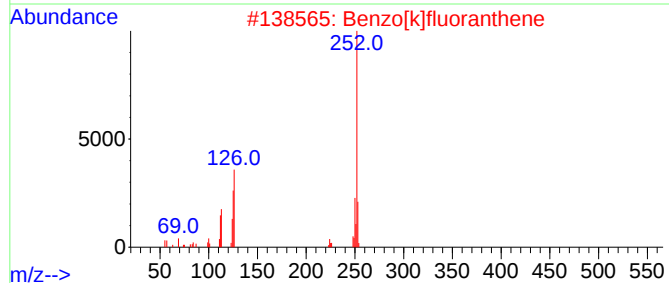
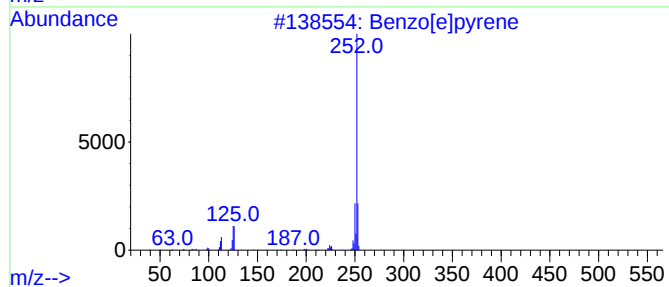
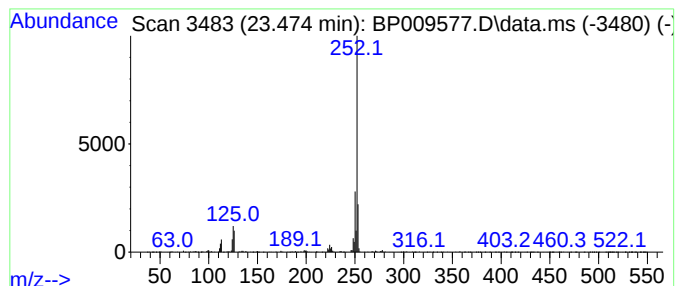
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.474	8.36 ng	1569360	Perylene-d12	23.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
4			Perylene	252	C20H12	000198-55-0	95
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP032822\
Data File : BP009577.D
Acq On : 28 Mar 2022 21:43
Operator : CG/JU
Sample : N2103-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CHRT-2001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.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...	3.023	14.2	ng	1208480	1	7.763	1698350	20.0
n-Hexadecanoic ...	18.086	5.3	ng	964925	4	17.175	3666950	20.0
4H-Cyclopenta[d...]	18.239	3.9	ng	719589	4	17.175	3666950	20.0
9,10-Dimethylan...	18.951	2.3	ng	414101	4	17.175	3666950	20.0
Octacosyl acetate	21.028	8.3	ng	2768030	5	21.292	6676950	20.0
Triphenylphosph...	21.410	2.7	ng	903881	5	21.292	6676950	20.0
Benzo[e]pyrene	23.474	8.4	ng	1569360	6	23.686	3756500	20.0