

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP032922\
 Data File : BP009598.D
 Acq On : 29 Mar 2022 17:24
 Operator : CG/JU
 Sample : N2095-15
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SB-15-5.0-6.0

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: BP009598.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.369	397	405	427	rBV	3948068	6798350	30.60%	6.046%
2	6.952	666	674	697	rBV	3755700	6931254	31.20%	6.165%
3	7.763	803	812	821	rBV	811845	1422031	6.40%	1.265%
4	8.916	997	1008	1022	rBV	2368107	4452199	20.04%	3.960%
5	10.551	1278	1286	1301	rBV	992201	1928000	8.68%	1.715%
6	13.028	1700	1707	1724	rBV	6291257	10037365	45.18%	8.927%
7	14.410	1935	1942	1959	rVB	1609752	2603133	11.72%	2.315%
8	15.910	2187	2197	2209	rBV	5229220	8175931	36.80%	7.272%
9	16.598	2307	2314	2319	rBV5	84878	244078	1.10%	0.217%
10	17.175	2406	2412	2418	rBV	1998399	3057785	13.76%	2.720%
11	17.592	2477	2483	2493	rBV	202568	388275	1.75%	0.345%
12	18.086	2562	2567	2573	rBV	542419	853885	3.84%	0.759%
13	18.145	2573	2577	2586	rVB	250038	413849	1.86%	0.368%
14	18.351	2608	2612	2617	rBV	275174	467512	2.10%	0.416%
15	18.416	2617	2623	2633	rVB2	296227	721804	3.25%	0.642%
16	19.022	2722	2726	2734	rVB3	148134	318287	1.43%	0.283%
17	19.204	2752	2757	2768	rBV	330908	543381	2.45%	0.483%
18	19.327	2772	2778	2789	rBV3	281605	806791	3.63%	0.718%
19	19.527	2808	2812	2813	rBV	192855	226761	1.02%	0.202%
20	19.557	2814	2817	2830	rVB	409588	756757	3.41%	0.673%
21	19.757	2845	2851	2871	rVB	12409861	16154277	72.71%	14.367%
22	20.439	2963	2967	2974	rBV	566823	757275	3.41%	0.674%
23	20.516	2976	2980	2984	rBV	363570	456246	2.05%	0.406%
24	21.027	3062	3067	3072	rBV2	551717	1080892	4.86%	0.961%
25	21.074	3072	3075	3082	rVB2	287122	476920	2.15%	0.424%
26	21.210	3094	3098	3105	rBV	742452	1072097	4.83%	0.954%
27	21.292	3105	3112	3116	rBV2	3844190	6060605	27.28%	5.390%
28	21.327	3116	3118	3125	rVV	908397	1261382	5.68%	1.122%
29	21.416	3127	3133	3151	rVV	13826321	22218154	100.00%	19.760%
30	22.133	3251	3255	3260	rVB	581037	804215	3.62%	0.715%
31	22.957	3390	3395	3399	rBV	1056946	2042940	9.19%	1.817%
32	23.004	3400	3403	3418	rVB	947502	1776642	8.00%	1.580%
33	23.533	3488	3493	3497	rBV2	458377	953646	4.29%	0.848%
34	23.580	3498	3501	3510	rVB2	719948	1471211	6.62%	1.308%
35	23.686	3512	3519	3531	rVB2	2132277	4703981	21.17%	4.184%

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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
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

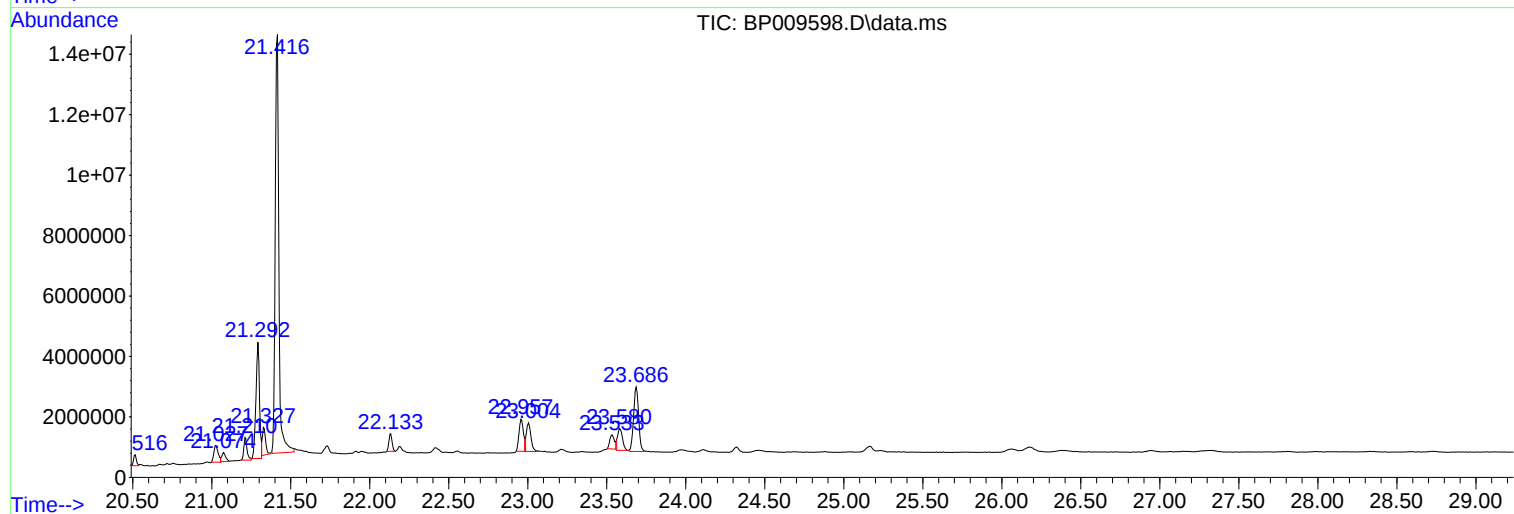
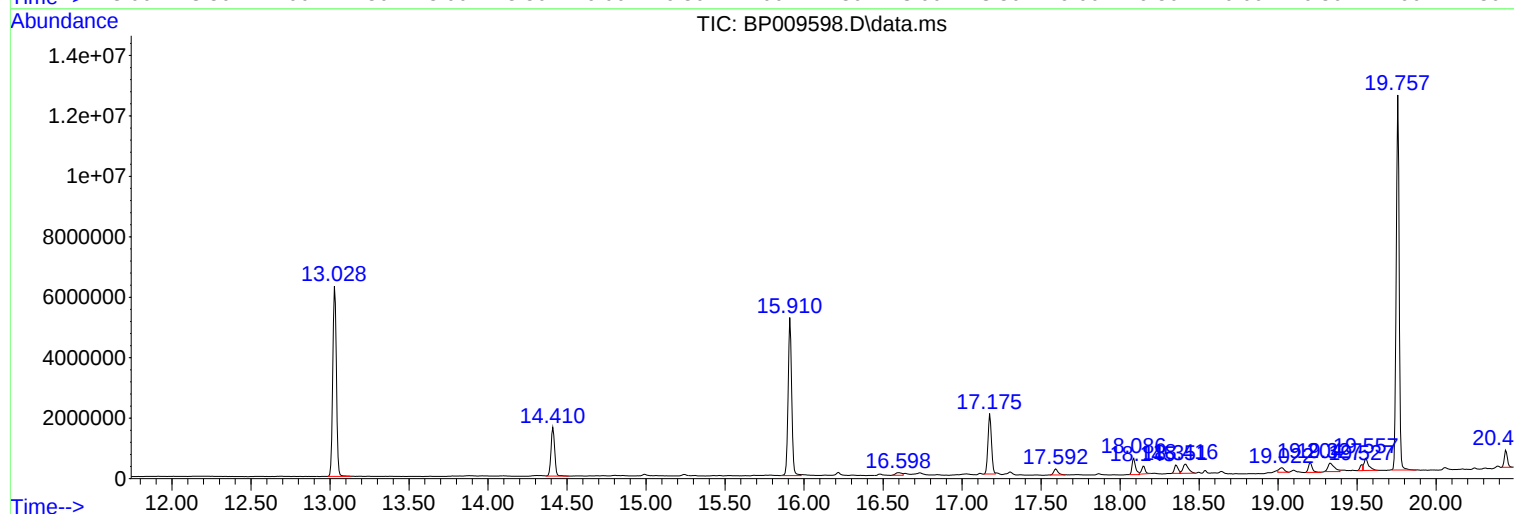
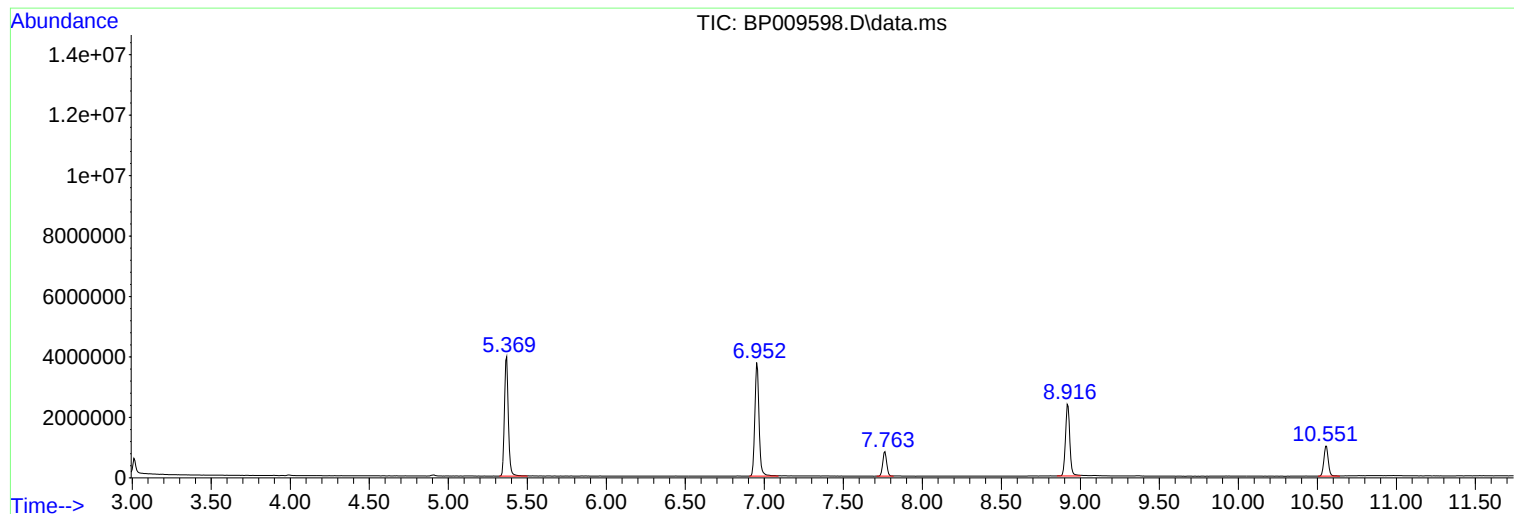
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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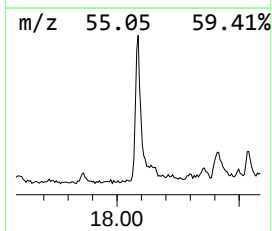
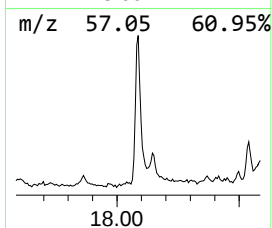
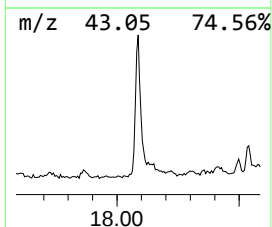
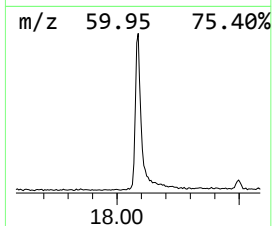
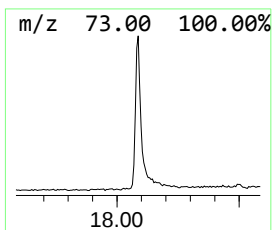
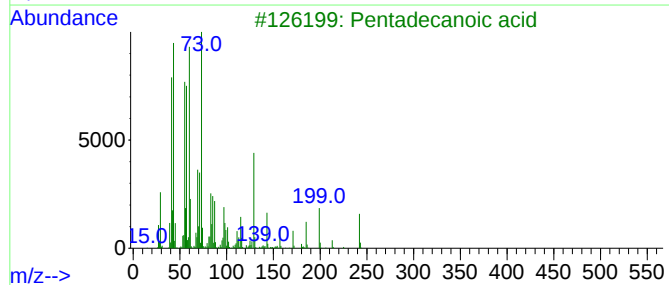
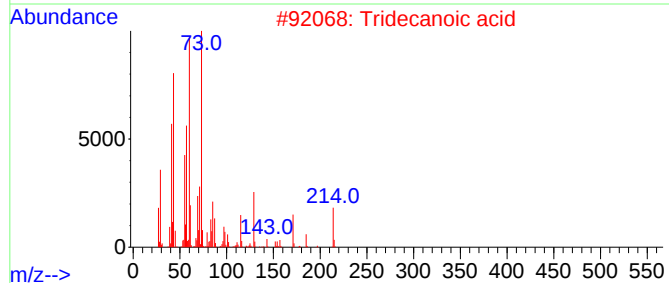
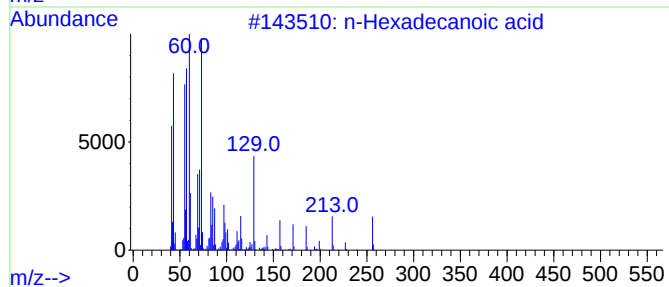
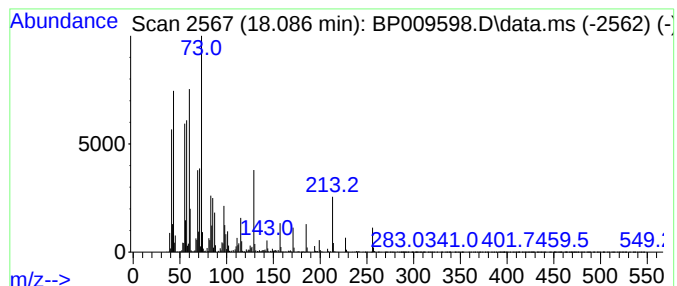
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.086	5.58 ng	853885	Phenanthrene-d10	17.175

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	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		n-Decanoic acid	172	C10H20O2	000334-48-5	70
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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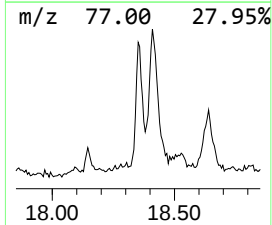
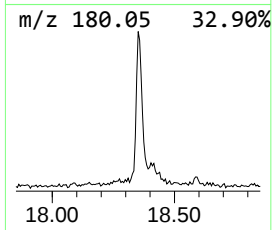
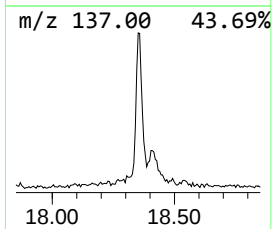
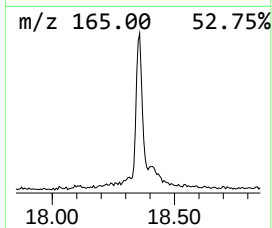
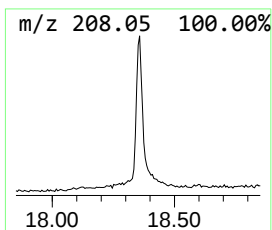
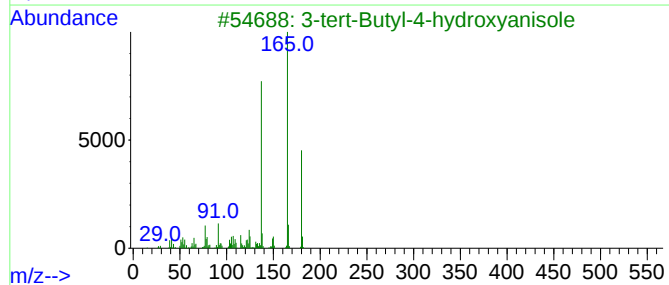
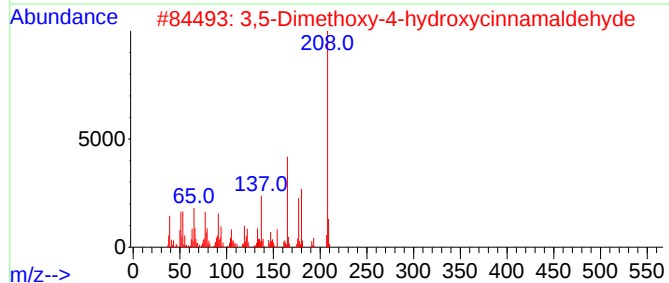
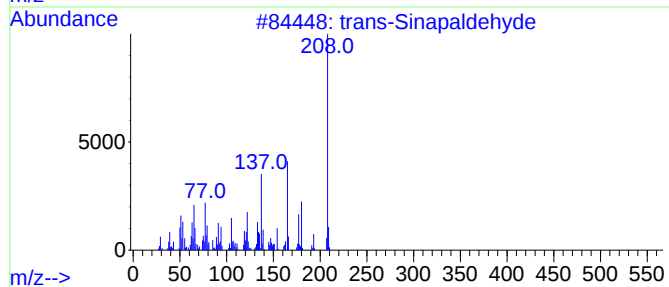
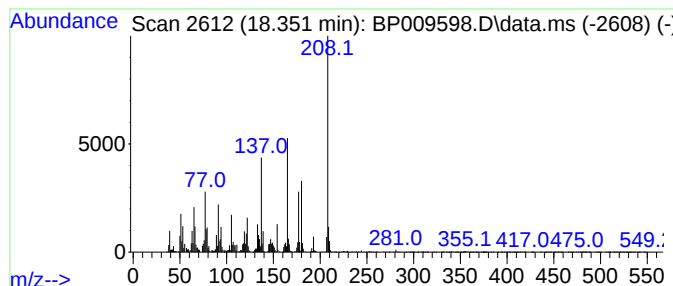
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 trans-Sinapaldehyde Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.351	3.06 ng	467512	Phenanthrene-d10	17.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Sinapaldehyde	208	C11H12O4	004206-58-0	98
2			3,5-Dimethoxy-4-hydroxycinnamal...	208	C11H12O4	087345-53-7	97
3			3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	80
4			2-Allyl-3-ethoxy-4-methoxyphenol	208	C12H16O3	1000122-70-6	62
5			1,2-Dimethoxy-4-(3-methoxy-1-pro...	208	C12H16O3	1000313-35-0	50



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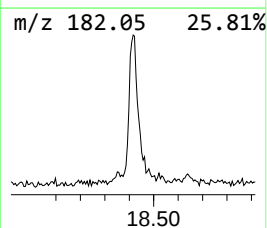
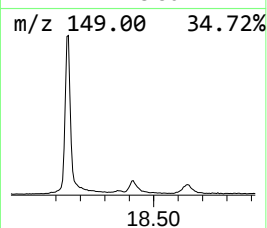
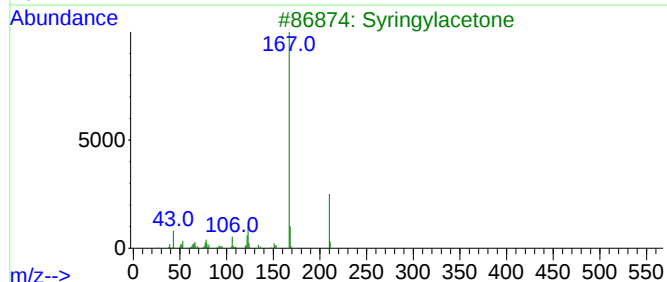
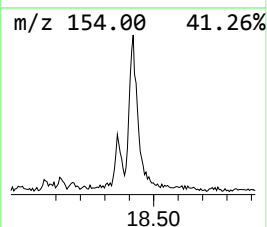
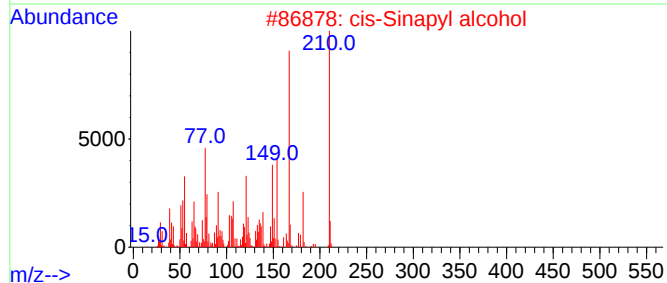
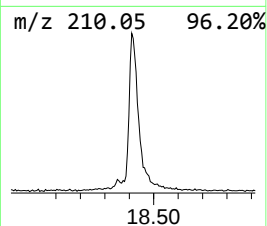
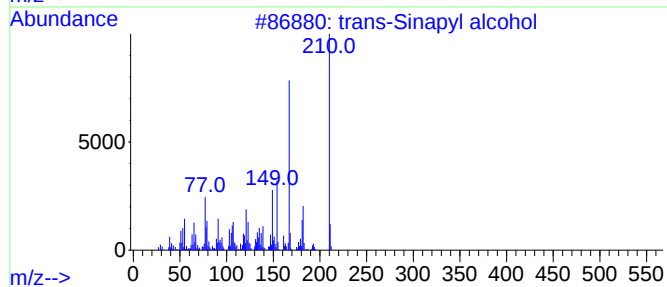
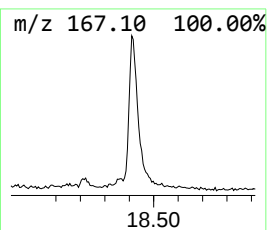
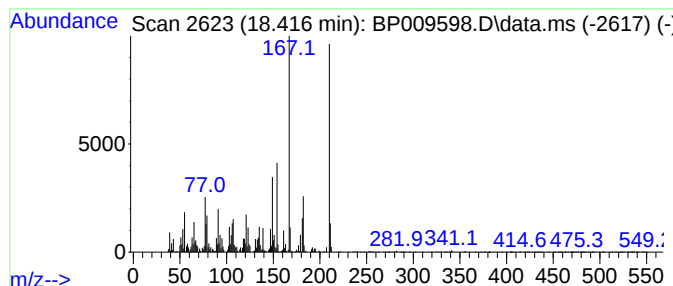
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 trans-Sinapyl alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.416	4.72 ng	721804	Phenanthrene-d10	17.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	99
2			cis-Sinapyl alcohol	210	C11H14O4	104330-63-4	90
3			Syringylacetone	210	C11H14O4	019037-58-2	60
4			1-Butyl-6,7-difluoro-1,3-benzimi...	210	C11H12F2N2	1375069-34-3	50
5			1-Butanone, 1-(2,4,6-trihydroxy-...	210	C11H14O4	001509-06-4	47



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ALS Vial : 4 Sample Multiplier: 1

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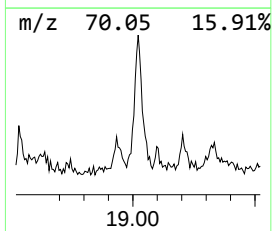
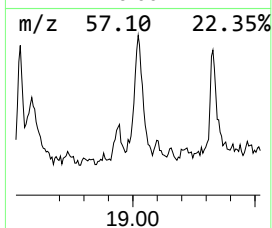
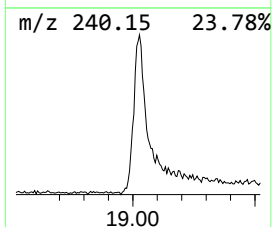
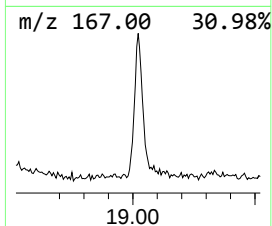
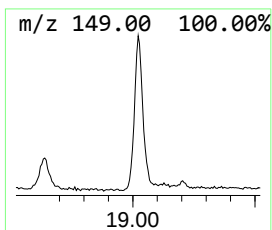
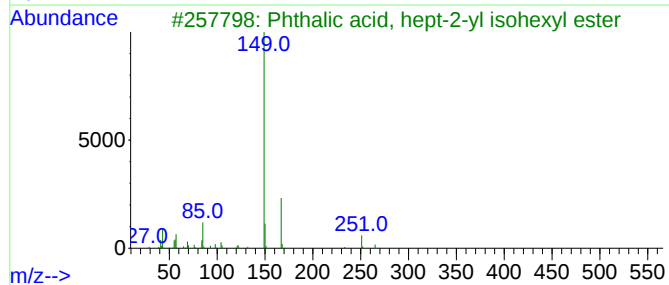
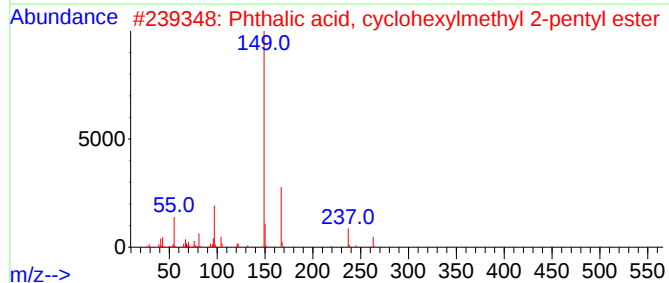
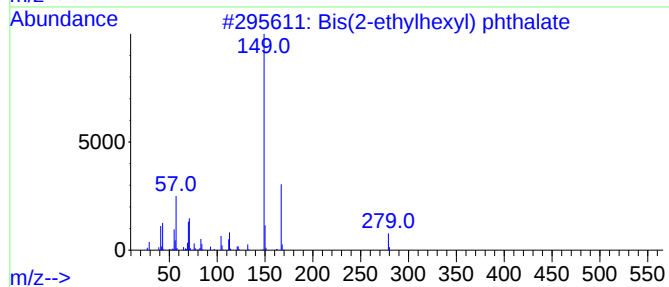
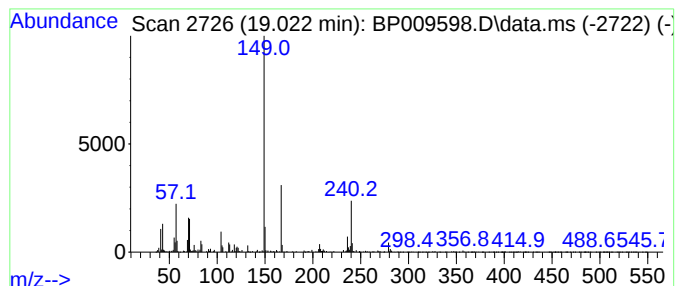
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Phthalic acid, cyclohexylme... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.022	2.08 ng	318287	Phenanthrene-d10	17.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	68
2			Phthalic acid, cyclohexylmethyl ...	332	C20H28O4	1000315-55-5	59
3			Phthalic acid, hept-2-yl isohexy...	348	C21H32O4	1000356-97-3	53
4			Phthalic acid, heptadecyl 2-prop...	516	C33H56O4	1000377-93-3	50
5			Phthalic acid, octyl 2-propylpen...	390	C24H38O4	1000377-92-4	50



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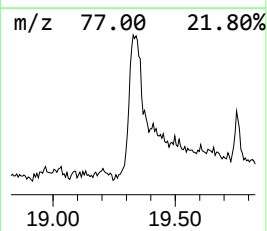
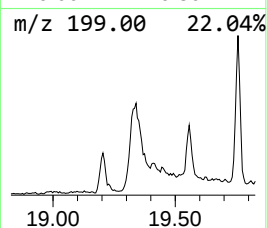
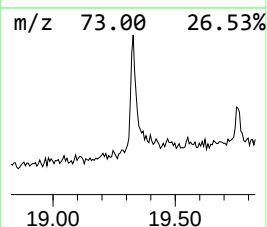
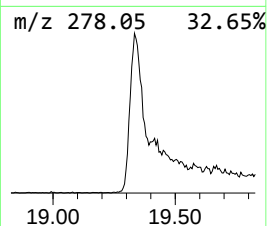
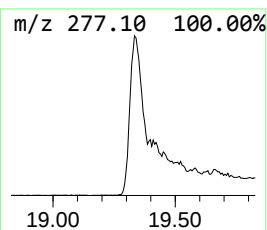
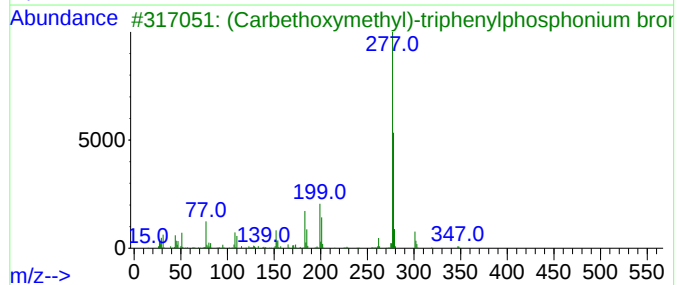
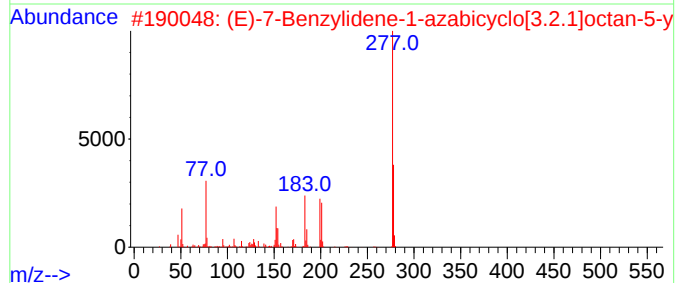
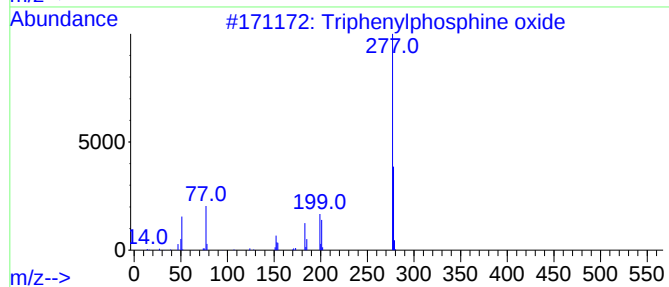
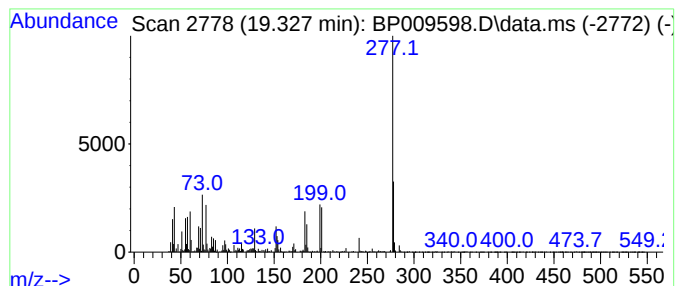
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.328	2.66 ng	806791	Chrysene-d12	21.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	64
3			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	59
4			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	47
5			Cobalt, (.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP032922\
Data File : BP009598.D
Acq On : 29 Mar 2022 17:24
Operator : CG/JU
Sample : N2095-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-15-5.0-6.0

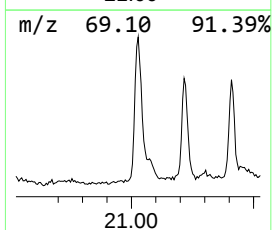
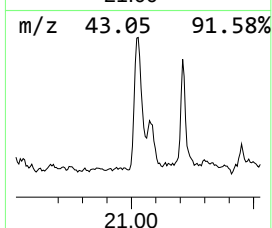
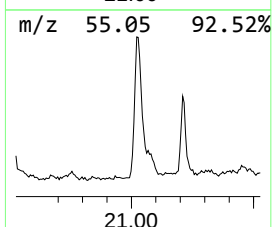
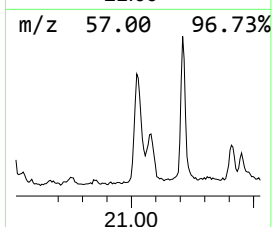
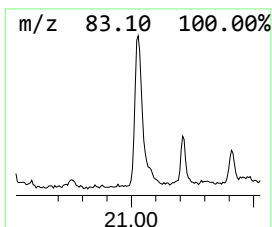
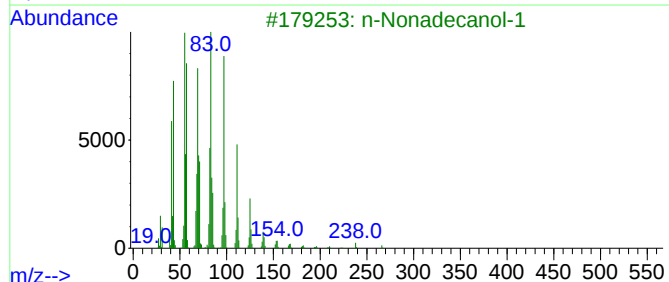
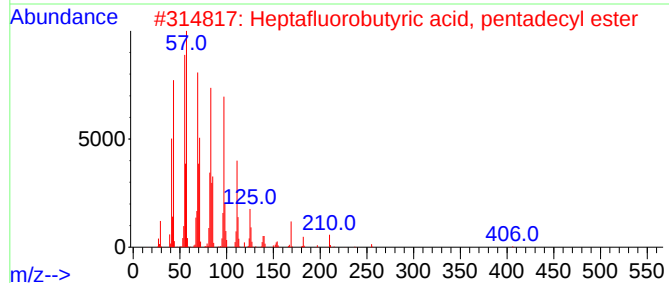
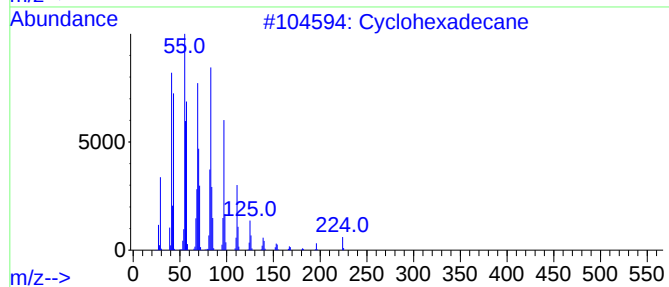
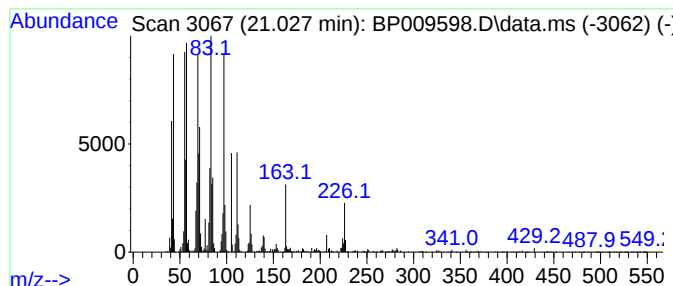
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.027	3.57 ng	1080890	Chrysene-d12	21.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	94
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	93
4			1-Heneicosanol	312	C21H44O	015594-90-8	93
5			Pentacos-1-ene	350	C25H50	016980-85-1	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP032922\
Data File : BP009598.D
Acq On : 29 Mar 2022 17:24
Operator : CG/JU
Sample : N2095-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-15-5.0-6.0

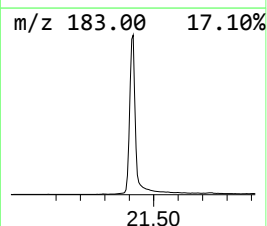
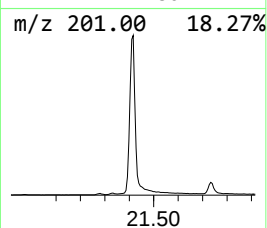
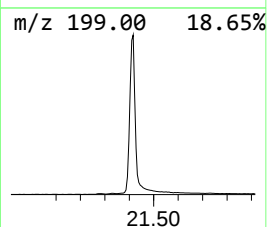
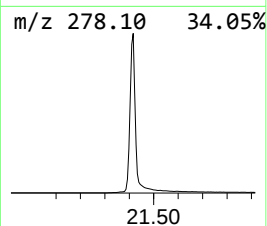
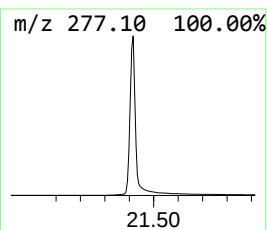
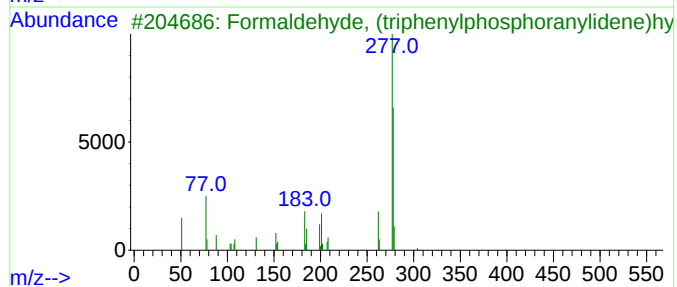
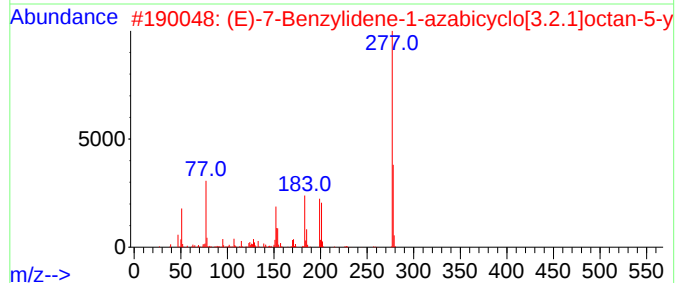
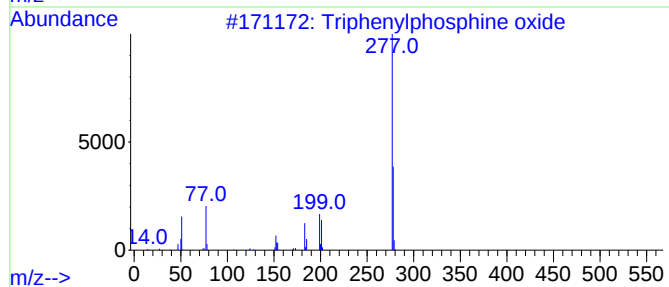
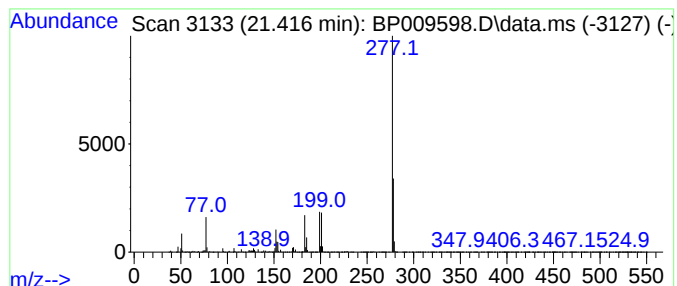
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 (E)-7-Benzylidene-1-azabicy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.416	73.32 ng	22218200	Chrysene-d12	21.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	47
4			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	28
5			Thiophene-3-carbonitrile, 4-(4-m...	277	C13H11NO2S2	1000268-75-0	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP032922\
Data File : BP009598.D
Acq On : 29 Mar 2022 17:24
Operator : CG/JU
Sample : N2095-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-15-5.0-6.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.086	5.6	ng	853885	4	17.175	3057790	20.0
trans-Sinapalde...	18.351	3.1	ng	467512	4	17.175	3057790	20.0
trans-Sinapyl a...	18.416	4.7	ng	721804	4	17.175	3057790	20.0
Phthalic acid, ...	19.022	2.1	ng	318287	4	17.175	3057790	20.0
Triphenylphosph...	19.328	2.7	ng	806791	5	21.292	6060610	20.0
Cyclohexadecane	21.027	3.6	ng	1080890	5	21.292	6060610	20.0
(E)-7-Benzylide...	21.416	73.3	ng	22218200	5	21.292	6060610	20.0