

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031723\
 Data File : BP014131.D
 Acq On : 17 Mar 2023 21:03
 Operator : CG/JU
 Sample : 01954-07
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SV-TP4-0316

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-BP030623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP014131.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.134	325	331	342	rBV	823038	1150779	19.50%	2.926%
2	5.605	404	411	427	rBV	1942173	2930511	49.65%	7.451%
3	7.222	678	686	697	rBV	1905079	3169570	53.70%	8.059%
4	8.058	817	828	836	rBV	501135	827917	14.03%	2.105%
5	9.234	1019	1028	1039	rBV	1190000	2017193	34.18%	5.129%
6	10.887	1302	1309	1316	rBV	677233	1142079	19.35%	2.904%
7	13.328	1716	1724	1737	rBV	2884393	4325342	73.28%	10.998%
8	13.969	1827	1833	1837	rBV	248078	355841	6.03%	0.905%
9	14.016	1837	1841	1847	rVB2	99335	160013	2.71%	0.407%
10	14.587	1929	1938	1947	rVB6	51523	139576	2.36%	0.355%
11	14.704	1951	1958	1965	rBV	1067738	1555888	26.36%	3.956%
12	15.987	2170	2176	2182	rBV	334826	457658	7.75%	1.164%
13	16.063	2183	2189	2194	rVV	165577	228367	3.87%	0.581%
14	16.198	2205	2212	2227	rBV	2783486	4006657	67.88%	10.187%
15	17.339	2402	2406	2414	rBV2	40770	72609	1.23%	0.185%
16	17.463	2421	2427	2432	rBV	1316500	1891352	32.04%	4.809%
17	17.504	2432	2434	2441	rVB	96826	131197	2.22%	0.334%
18	18.322	2568	2573	2579	rBV	745557	1013787	17.18%	2.578%
19	19.463	2762	2767	2772	rVB	319810	462707	7.84%	1.176%
20	19.551	2778	2782	2788	rBV	224828	356303	6.04%	0.906%
21	19.816	2823	2827	2835	rVB	290511	407512	6.90%	1.036%
22	19.998	2853	2858	2865	rBV	4783143	5902455	100.00%	15.008%
23	20.628	2961	2965	2969	rBV	808458	953516	16.15%	2.424%
24	20.663	2969	2971	2979	rVB4	130057	192647	3.26%	0.490%
25	21.216	3061	3065	3071	rBV	691304	814941	13.81%	2.072%
26	21.428	3097	3101	3105	rVB	450577	553507	9.38%	1.407%
27	21.545	3116	3121	3126	rBV	1550939	2203765	37.34%	5.603%
28	24.080	3547	3552	3559	rVB2	954325	1905978	32.29%	4.846%

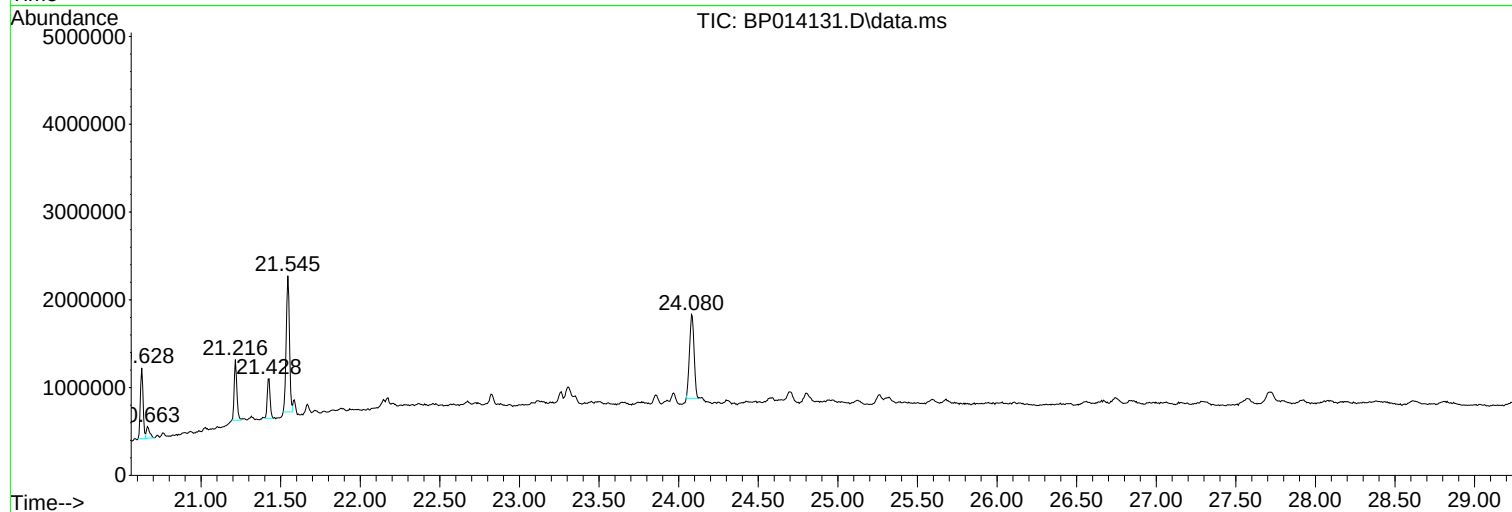
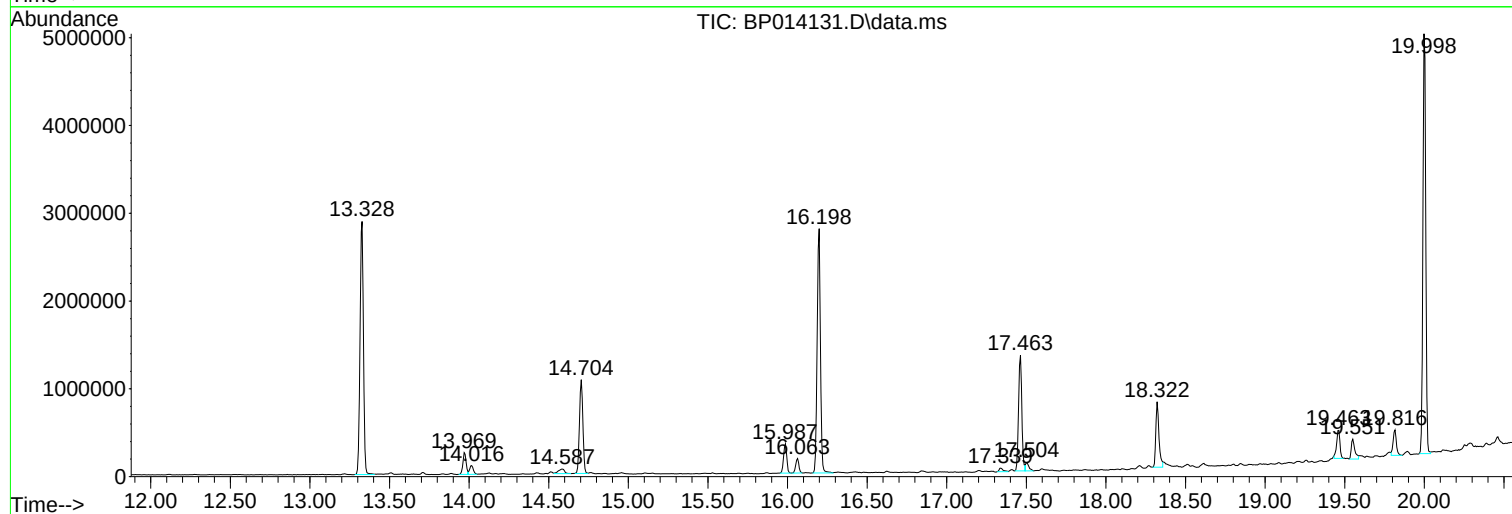
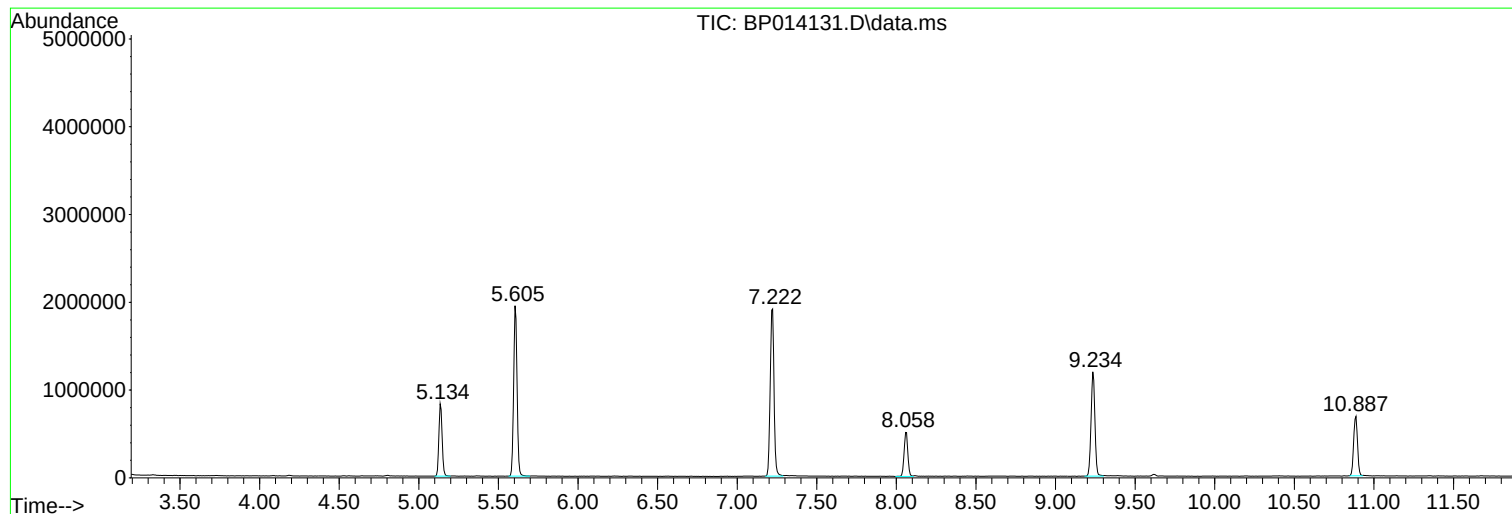
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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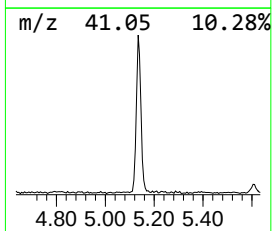
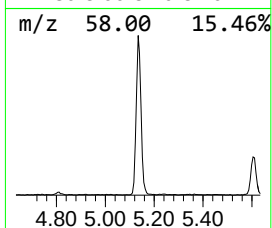
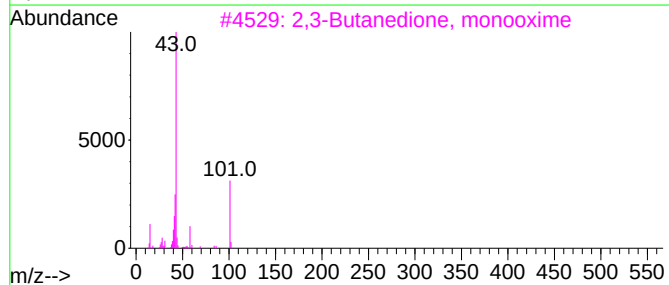
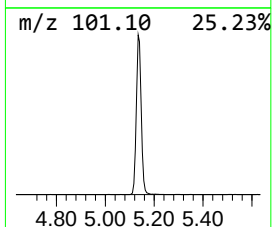
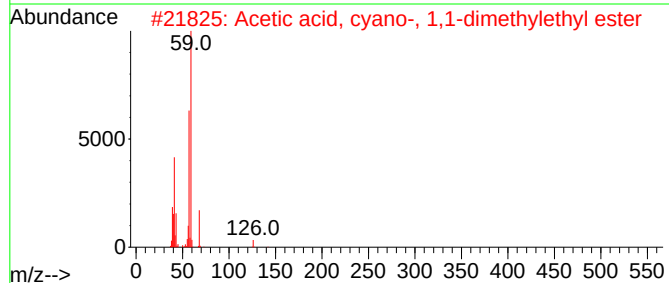
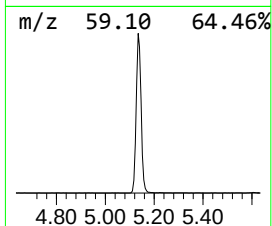
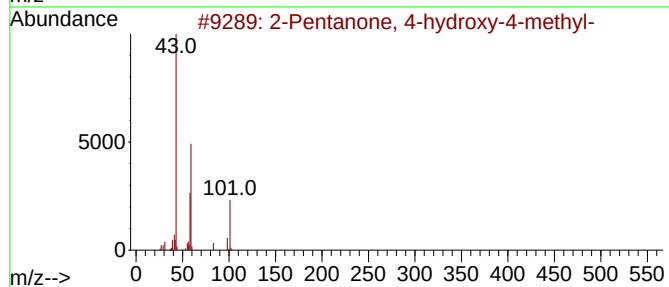
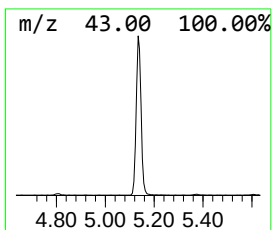
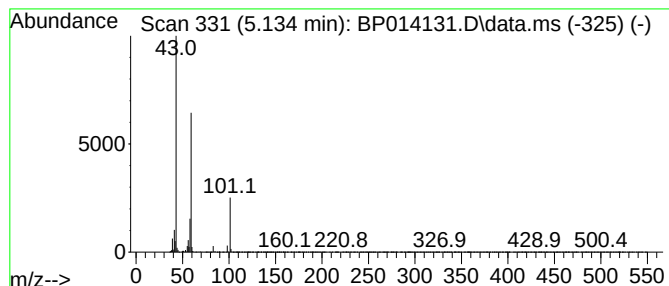
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.134	27.80 ng	1150780	1,4-Dichlorobenzene-d4	8.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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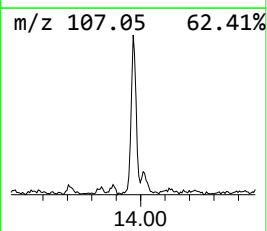
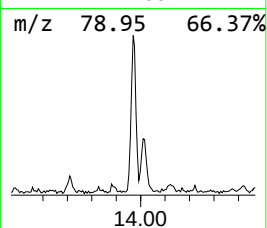
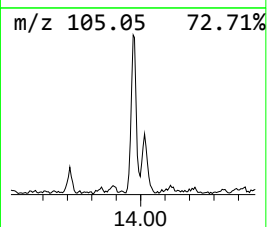
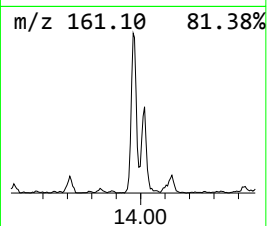
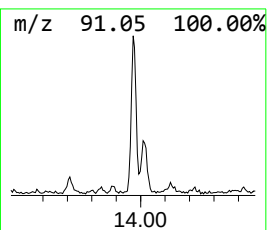
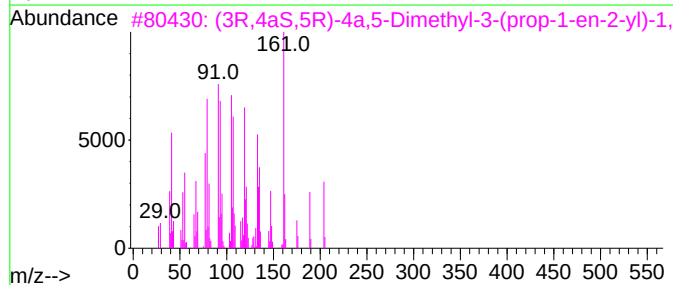
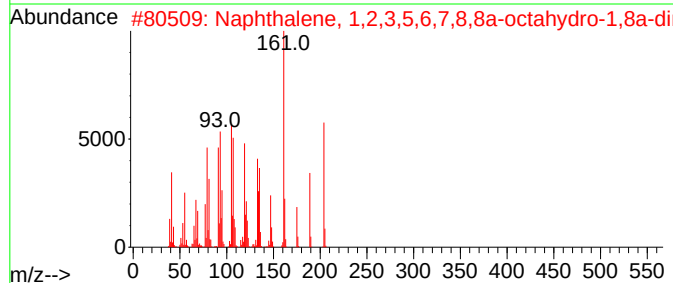
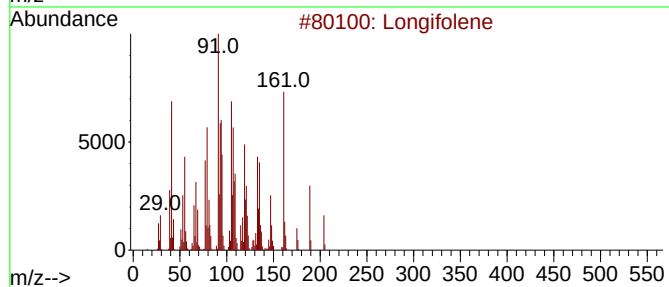
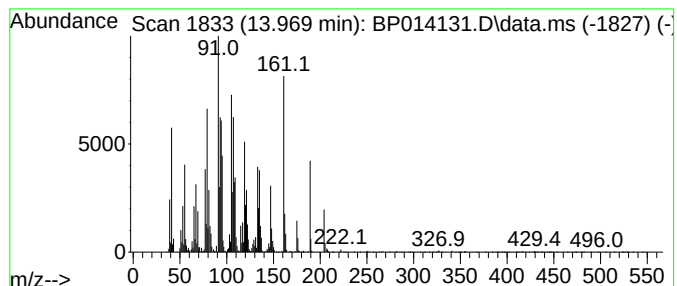
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Longifolene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.969	4.57 ng	355841	Acenaphthene-d10	14.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Longifolene	204	C15H24	000475-20-7	99
2			Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	97
3			(3R,4aS,5R)-4a,5-Dimethyl-3-(pro...	204	C15H24	024741-64-8	96
4			Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	010219-75-7	95
5			Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	000483-75-0	90



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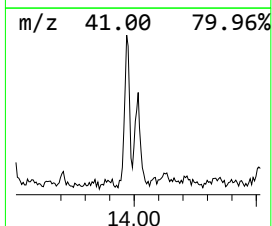
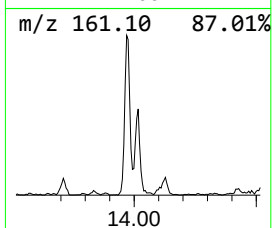
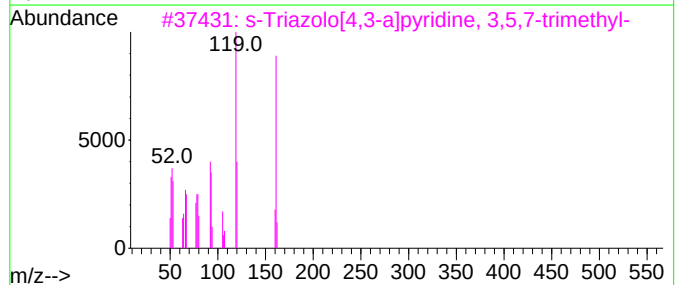
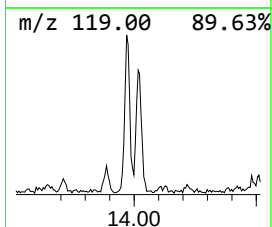
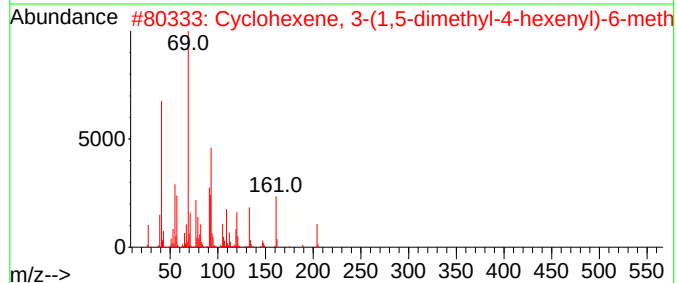
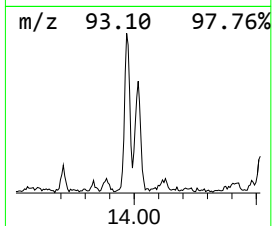
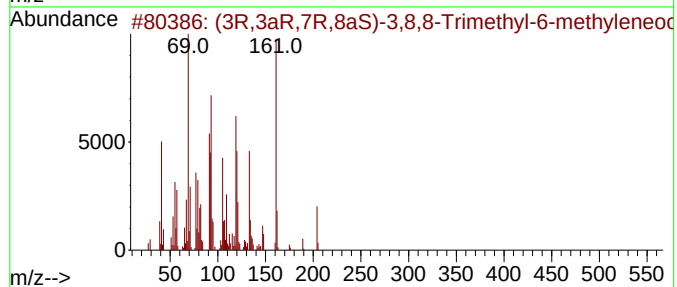
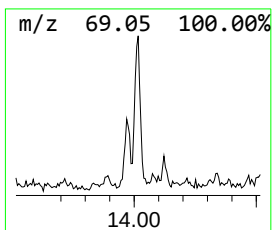
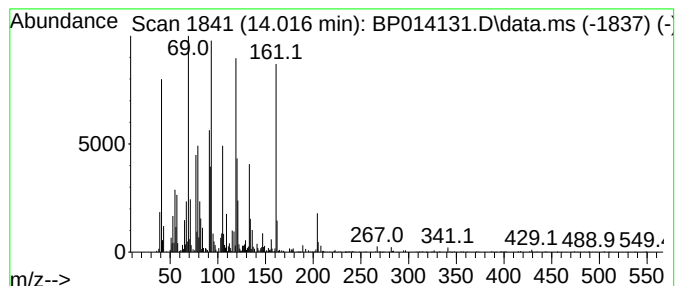
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TIC Integration Parameters: LSCINT.P

Peak Number 3 (3R,3aR,7R,8aS)-3,8,8-Trime... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD			R.T.
14.016	2.06 ng	160013	Acenaphthene-d10			14.704
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	(3R,3aR,7R,8aS)-3,8,8-Trimethyl-...		204	C15H24	079120-98-2	70
2	Cyclohexene, 3-(1,5-dimethyl-4-h...		204	C15H24	020307-83-9	64
3	s-Triazolo[4,3-a]pyridine, 3,5,7...		161	C9H11N3	004919-15-7	46
4	Copaene		204	C15H24	003856-25-5	46
5	.alpha.-Cubebene		204	C15H24	017699-14-8	30



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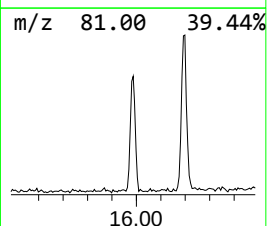
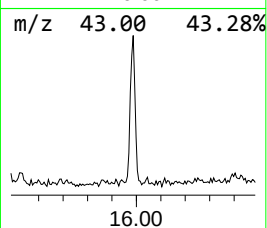
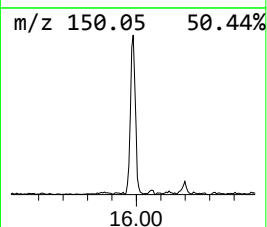
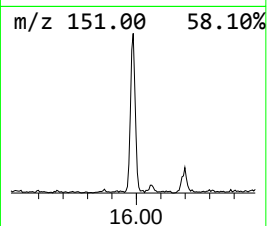
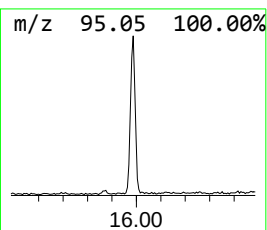
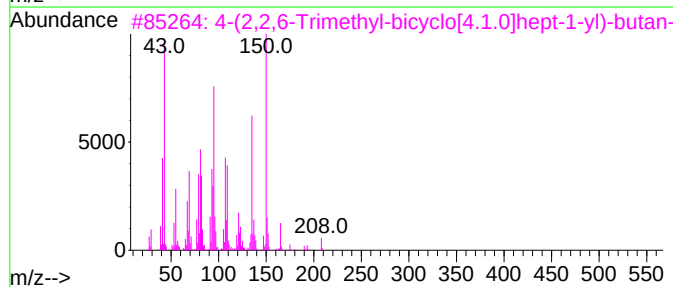
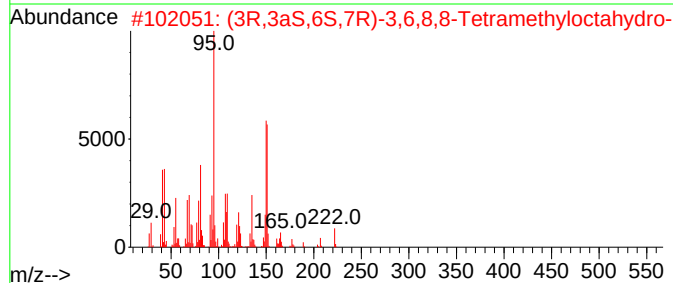
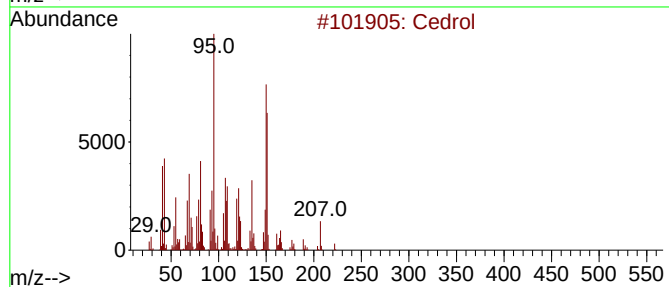
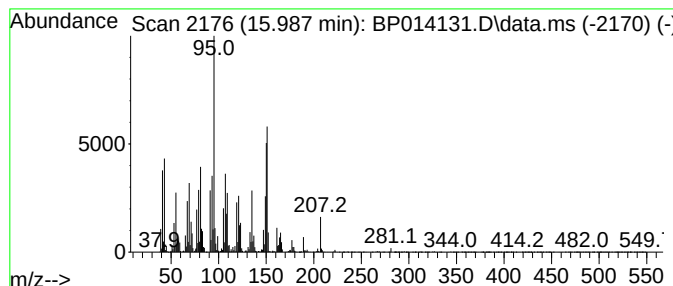
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Peak Number 4 Cedrol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.987	5.88 ng	457658	Acenaphthene-d10	14.704	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cedrol	222	C15H26O	000077-53-2	91
2	(3R,3aS,6S,7R)-3,6,8,8-Tetrameth...	222	C15H26O	019903-73-2	80
3	4-(2,2,6-Trimethyl-bicyclo[4.1.0...	208	C14H24O	077143-20-5	49
4	1,4 Benzodioxan-6-amine	151	C8H9NO2	022013-33-8	30
5	Piperonylamine	151	C8H9NO2	002620-50-0	30



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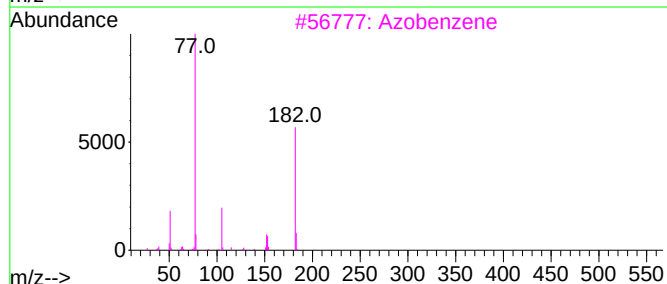
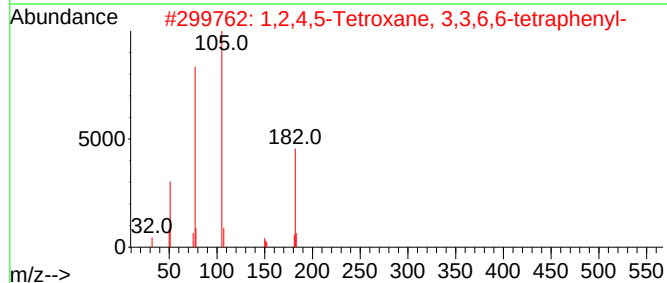
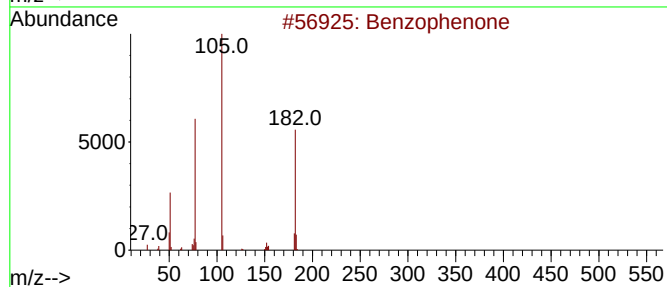
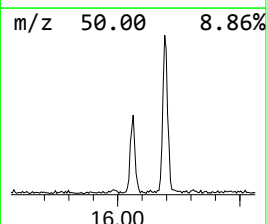
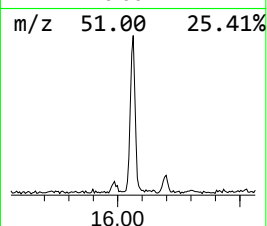
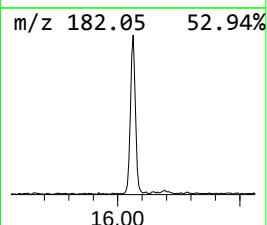
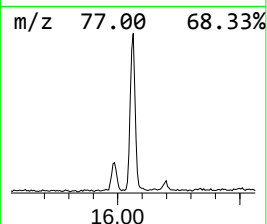
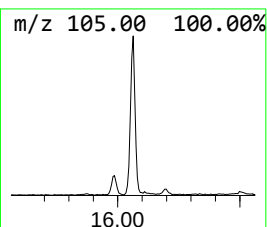
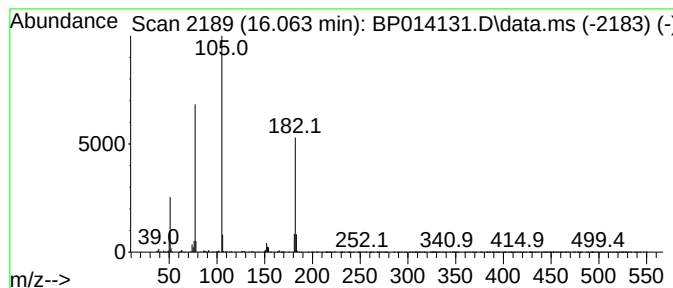
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.063	2.94 ng	228367	Acenaphthene-d10	14.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3			Azobenzene	182	C12H10N2	000103-33-3	64
4			Azobenzene, (E)-	182	C12H10N2	017082-12-1	59
5			1,1-Diphenyl-2-phenylthiobut-3-e...	332	C22H20OS	097370-20-2	45



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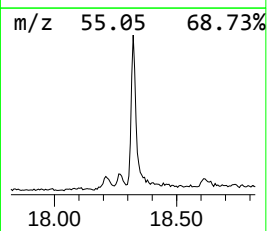
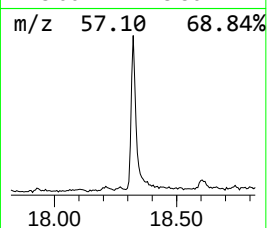
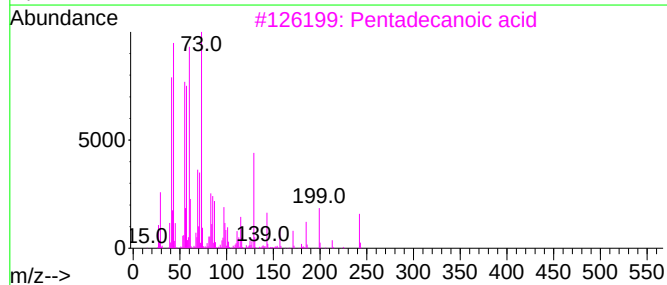
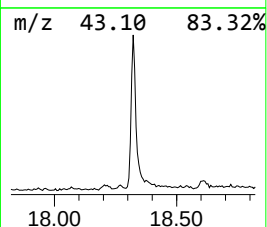
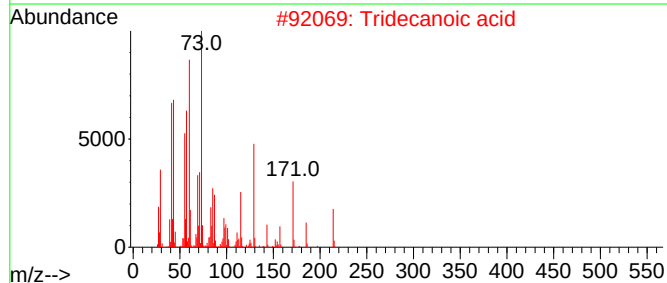
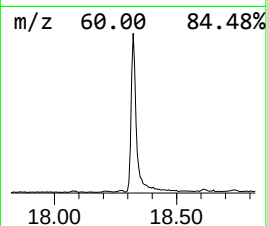
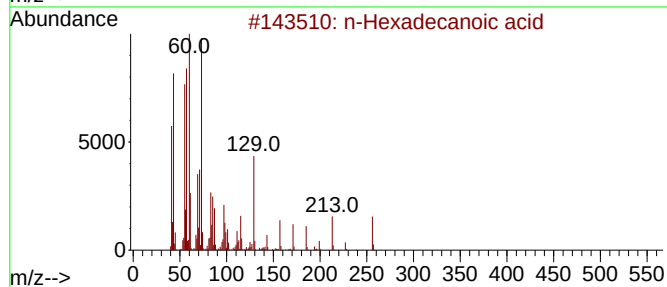
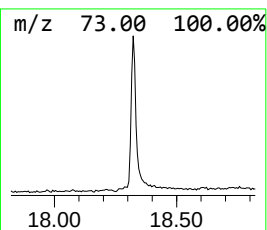
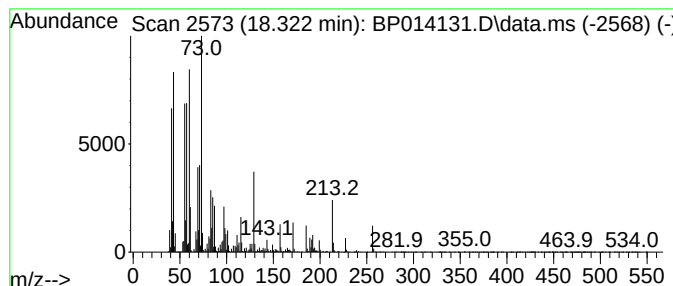
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.322	10.72 ng	1013790	Phenanthrene-d10	17.463

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	91
4			Octadecanoic acid	284	C18H36O2	000057-11-4	87
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031723\
Data File : BP014131.D
Acq On : 17 Mar 2023 21:03
Operator : CG/JU
Sample : 01954-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SV-TP4-0316

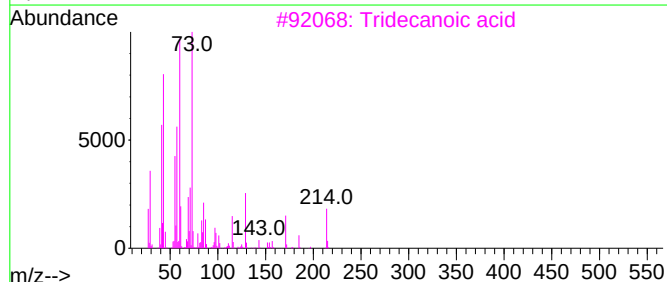
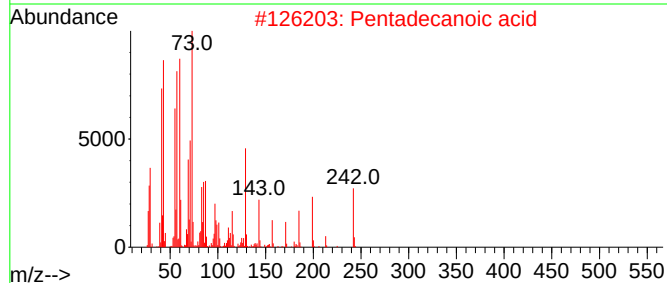
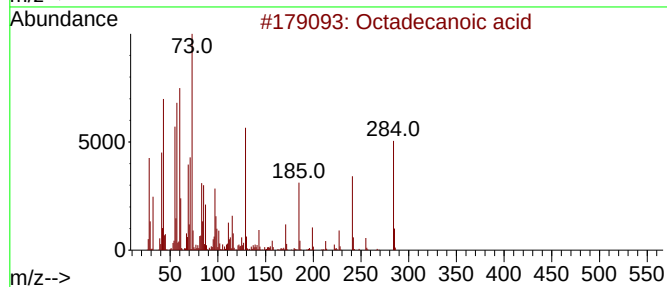
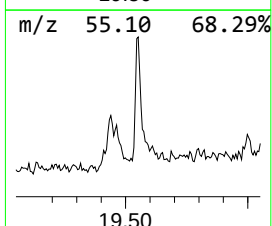
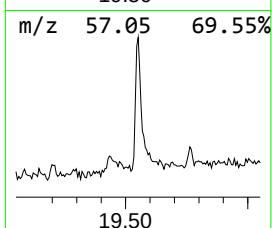
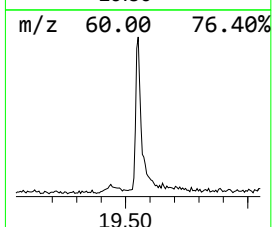
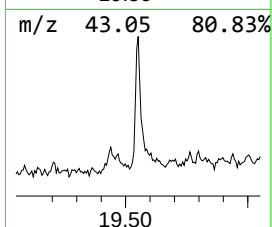
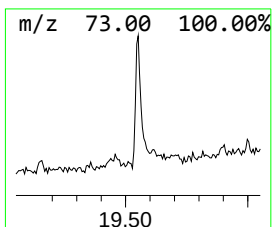
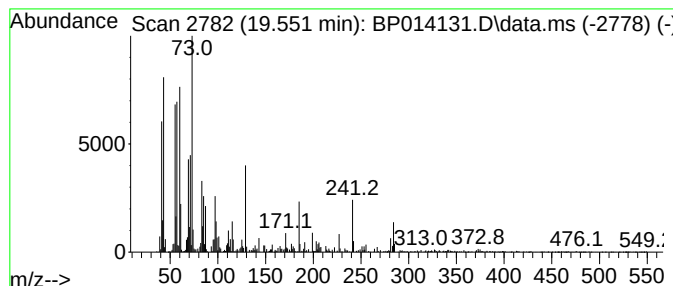
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.551	3.23 ng	356303	Chrysene-d12	21.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	76
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031723\
Data File : BP014131.D
Acq On : 17 Mar 2023 21:03
Operator : CG/JU
Sample : 01954-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

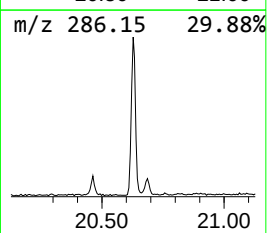
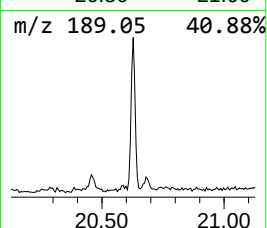
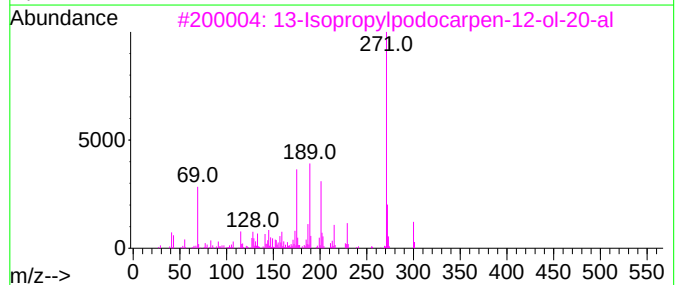
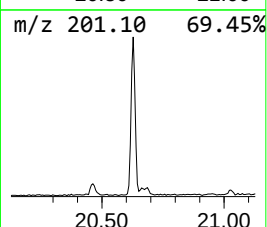
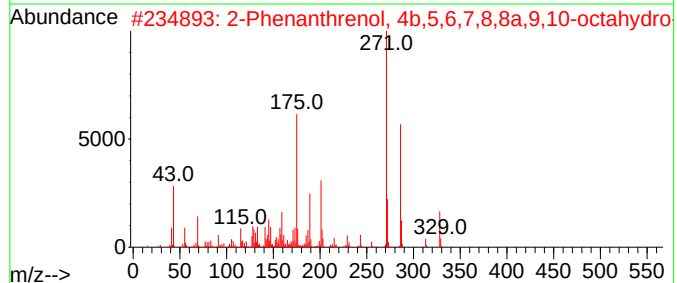
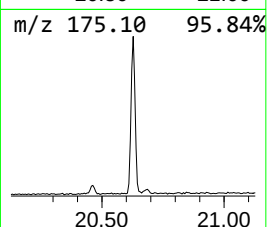
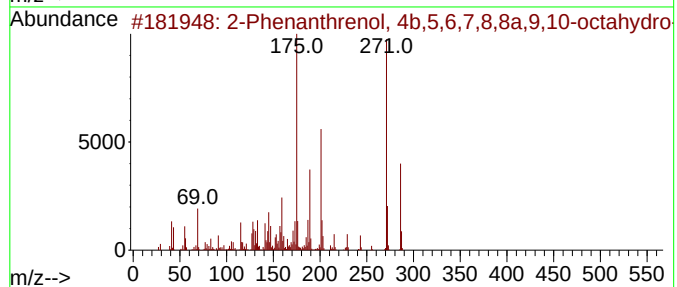
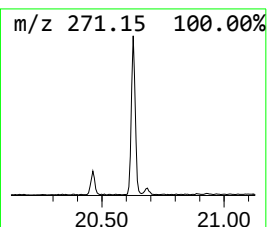
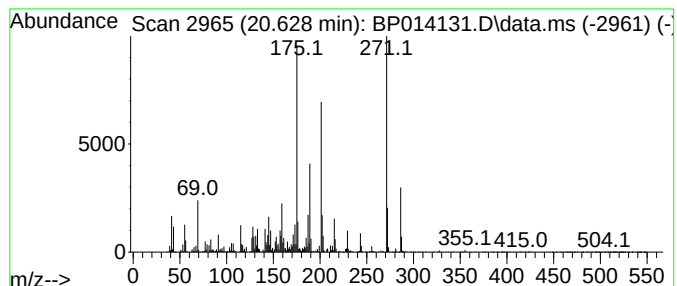
Instrument :
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ClientSampleId :
SV-TP4-0316

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.628	8.65 ng	953516	Chrysene-d12	21.545	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	99
2	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	328	C22H32O2	015340-82-6	87
3	13-Isopropylpodocarpin-12-ol-20-al	300	C20H28O2	024035-37-8	47
4	(4Br,8As)-(+)-4B,5,6,7,8,8A,9,10...	346	C22H34O3	1000426-72-2	43
5	Podocarpa-8,11,13-trien-17-oic a...	344	C22H32O3	024067-43-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031723\
Data File : BP014131.D
Acq On : 17 Mar 2023 21:03
Operator : CG/JU
Sample : 01954-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SV-TP4-0316

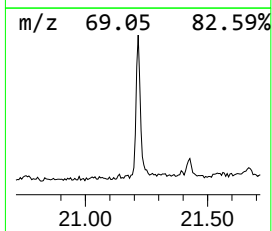
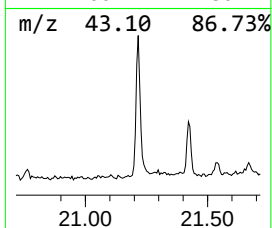
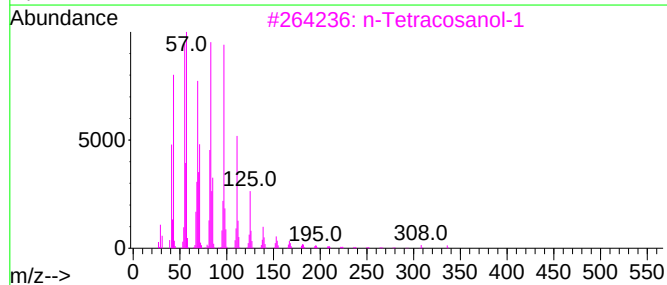
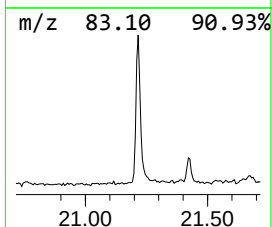
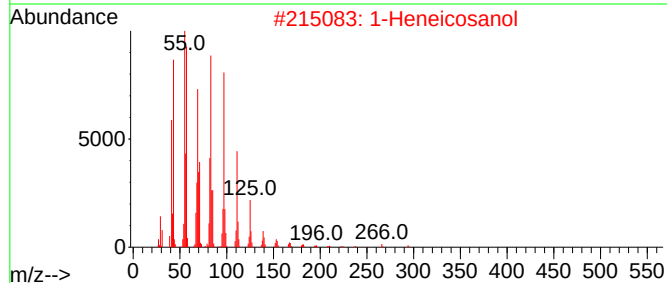
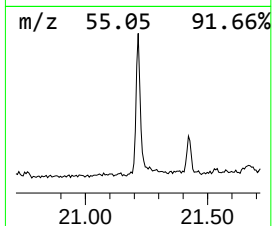
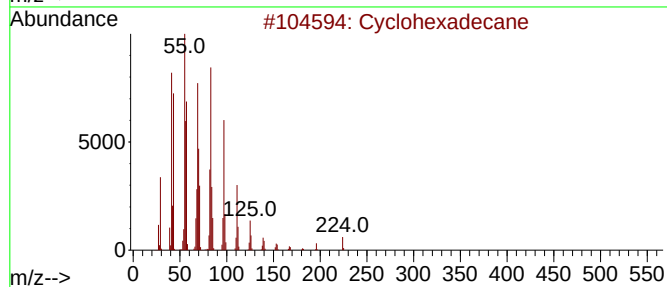
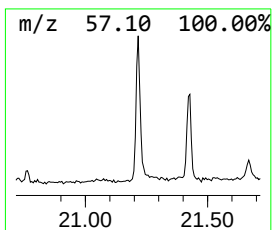
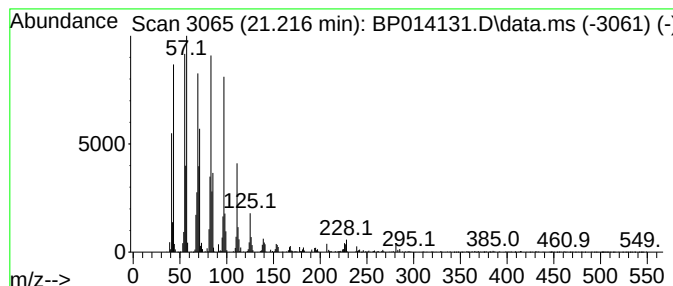
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.216	7.40 ng	814941	Chrysene-d12	21.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	94
2			1-Heneicosanol	312	C21H44O	015594-90-8	94
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4			Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	94
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031723\
Data File : BP014131.D
Acq On : 17 Mar 2023 21:03
Operator : CG/JU
Sample : 01954-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SV-TP4-0316

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030623.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
2-Pentanone, 4-...	5.134	27.8	ng	1150780	1	8.063	827917	20.0
Longifolene	13.969	4.6	ng	355841	3	14.704	1555890	20.0
(3R,3aR,7R,8aS)...	14.016	2.1	ng	160013	3	14.704	1555890	20.0
Cedrol	15.987	5.9	ng	457658	3	14.704	1555890	20.0
Benzophenone	16.063	2.9	ng	228367	3	14.704	1555890	20.0
n-Hexadecanoic ...	18.322	10.7	ng	1013790	4	17.463	1891350	20.0
Octadecanoic acid	19.551	3.2	ng	356303	5	21.545	2203770	20.0
2-Phenanthrenol...	20.628	8.7	ng	953516	5	21.545	2203770	20.0
Cyclohexadecane	21.216	7.4	ng	814941	5	21.545	2203770	20.0