

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082024\
Data File : BP021589.D
Acq On : 21 Aug 2024 02:44
Operator : RC/JU
Sample : P3657-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
917-J-WS-081624

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-BP081324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP021589.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.028	3	7	27	rVB	10419953	13090411	50.65%	11.246%
2	5.405	401	411	419	rBV	2745850	4070346	15.75%	3.497%
3	6.969	669	677	688	rBV	1783448	2833856	10.97%	2.435%
4	7.805	812	819	827	rBV	1306164	2109651	8.16%	1.812%
5	8.958	1005	1015	1024	rBV	3615061	6100027	23.60%	5.241%
6	10.599	1282	1294	1307	rBV	1839557	3089592	11.95%	2.654%
7	11.334	1413	1419	1424	rBV	216485	363595	1.41%	0.312%
8	13.063	1706	1713	1734	rBV	9425361	14116289	54.62%	12.128%
9	14.457	1943	1950	1956	rBV	3240496	4204194	16.27%	3.612%
10	15.975	2201	2208	2222	rBV	9684629	14151982	54.76%	12.158%
11	17.269	2421	2428	2436	rVB	3053383	5194153	20.10%	4.462%
12	17.345	2437	2441	2445	rBV	211260	286922	1.11%	0.247%
13	18.216	2582	2589	2595	rBV	762739	1463670	5.66%	1.257%
14	18.416	2611	2623	2627	rBV4	887705	2771662	10.72%	2.381%
15	18.469	2630	2632	2635	rVB2	245416	325559	1.26%	0.280%
16	18.757	2677	2681	2686	rBV2	324954	657456	2.54%	0.565%
17	18.951	2711	2714	2719	rVB	250748	343393	1.33%	0.295%
18	19.316	2772	2776	2780	rBV2	186997	299508	1.16%	0.257%
19	19.533	2807	2813	2819	rVB3	528993	1145349	4.43%	0.984%
20	19.992	2885	2891	2896	rVB	20610114	25844330	100.00%	22.203%
21	20.216	2927	2929	2931	rBV2	399280	412667	1.60%	0.355%
22	21.092	3074	3078	3084	rBV4	305715	650204	2.52%	0.559%
23	21.404	3126	3131	3136	rBV3	769924	1496689	5.79%	1.286%
24	21.727	3180	3186	3193	rVB2	3286014	5504103	21.30%	4.729%
25	25.168	3763	3771	3782	rVB2	1882754	5872027	22.72%	5.045%

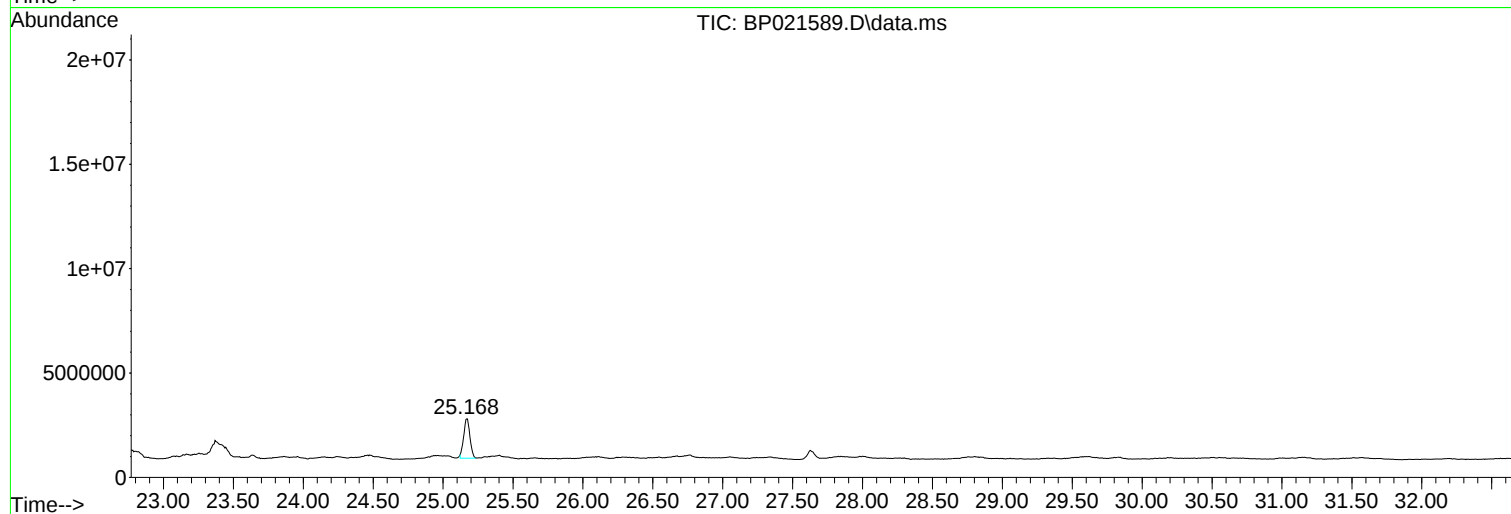
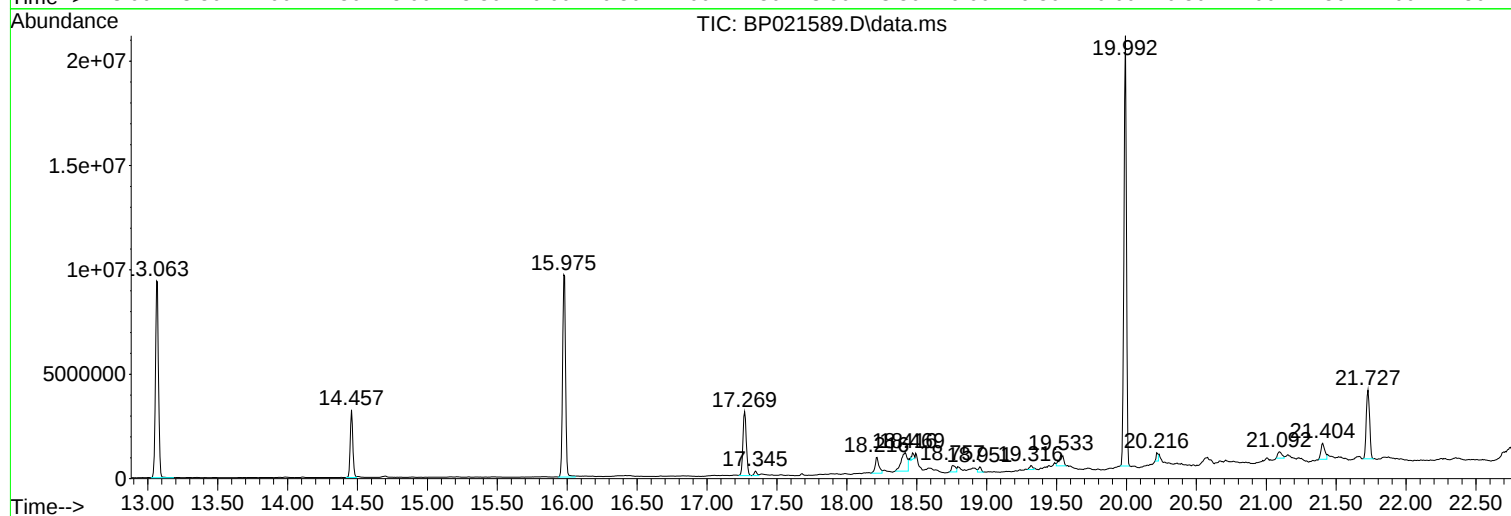
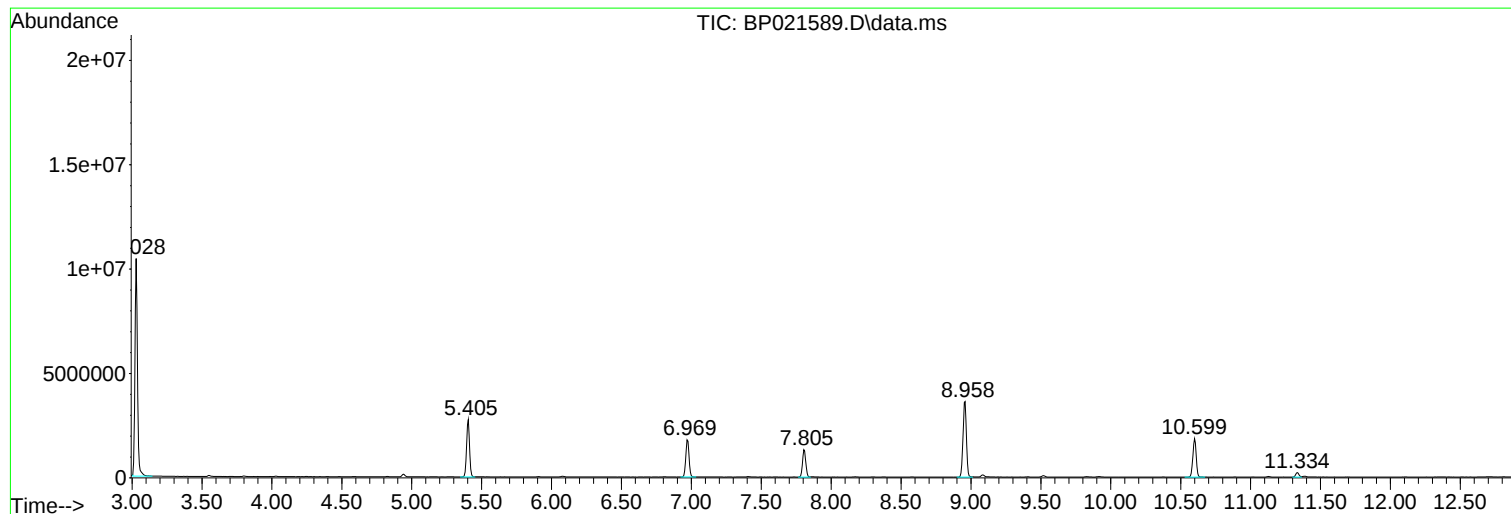
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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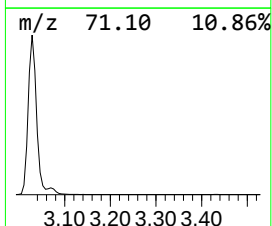
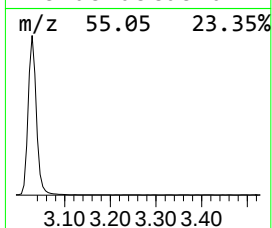
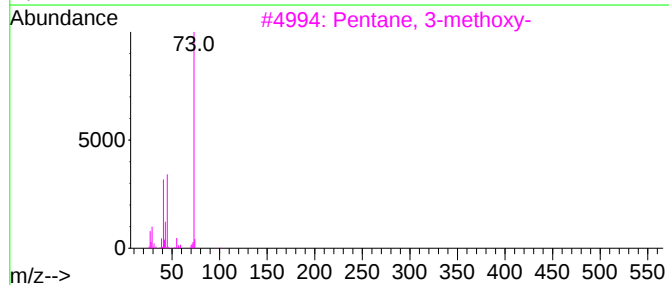
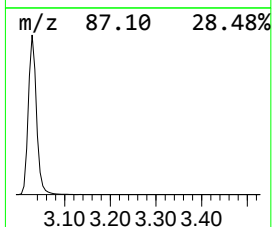
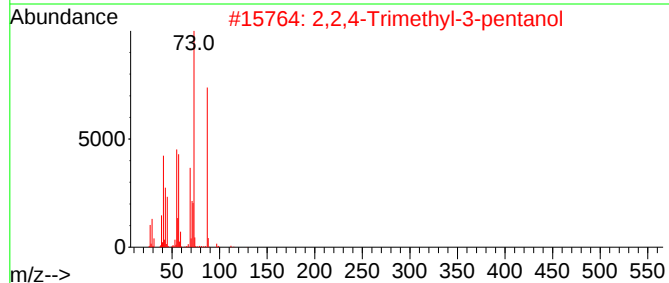
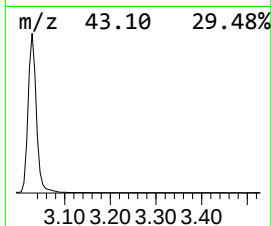
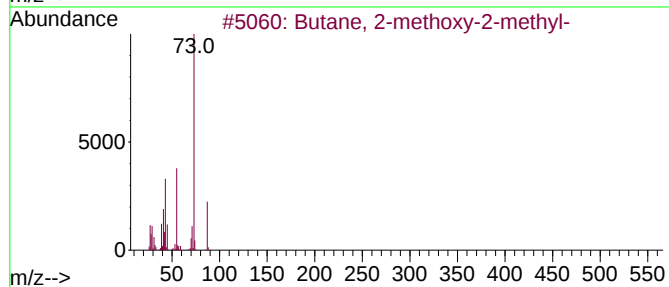
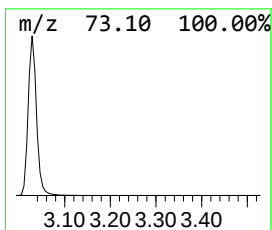
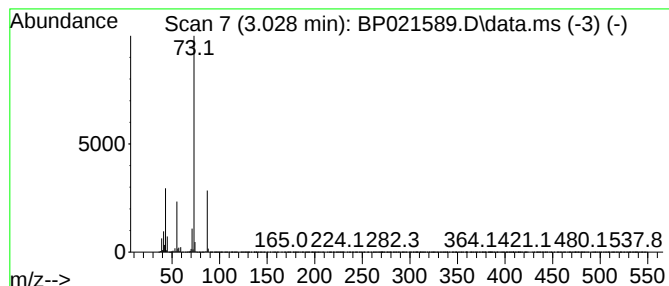
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.028	124.10 ng	13090400	1,4-Dichlorobenzene-d4	7.805

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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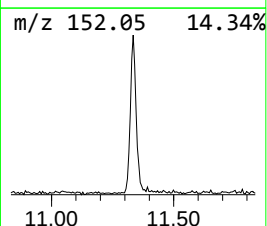
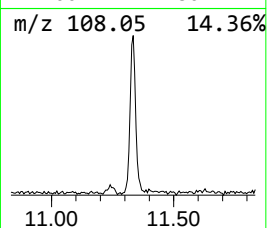
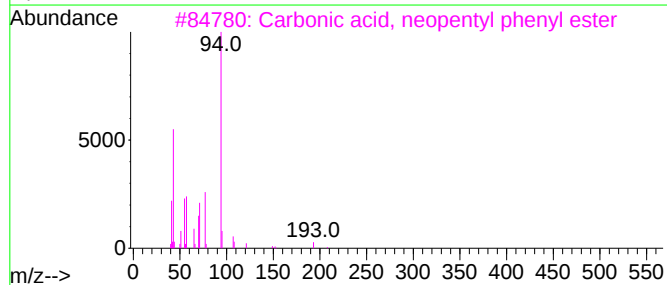
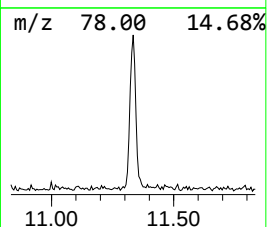
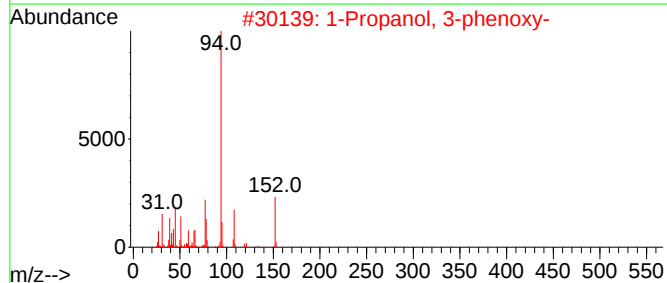
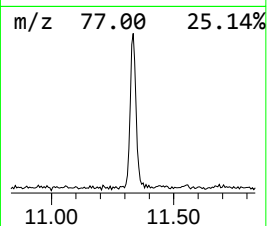
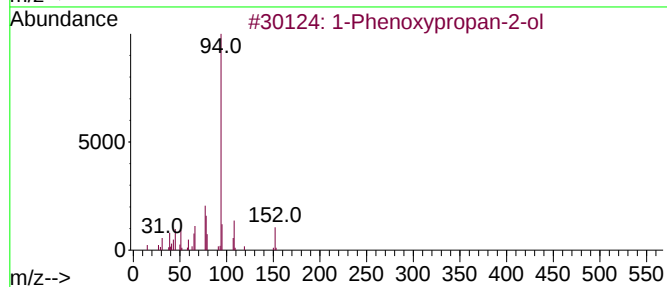
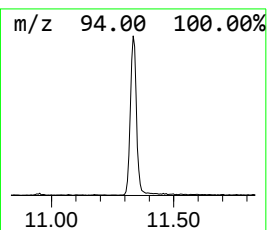
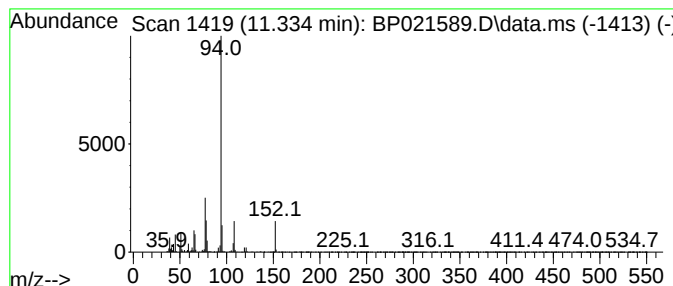
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Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.334	2.35 ng	363595	Naphthalene-d8	10.599

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
4			Carbonic acid, sec-butyl phenyl ...	194	C11H14O3	013183-17-0	59
5			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	58



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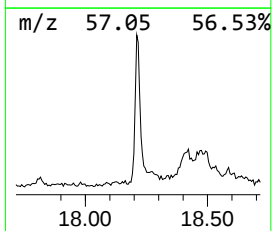
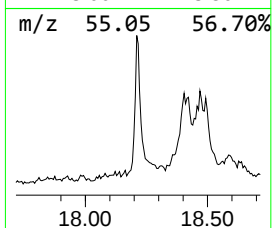
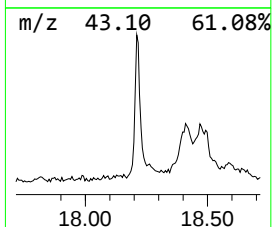
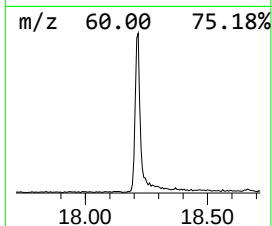
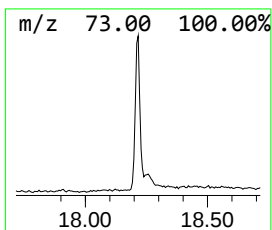
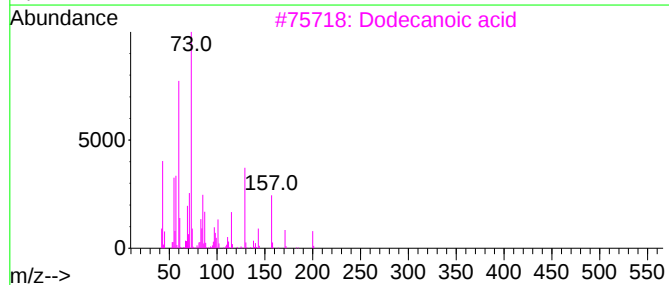
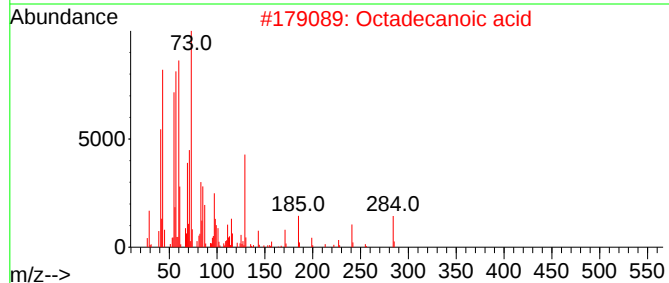
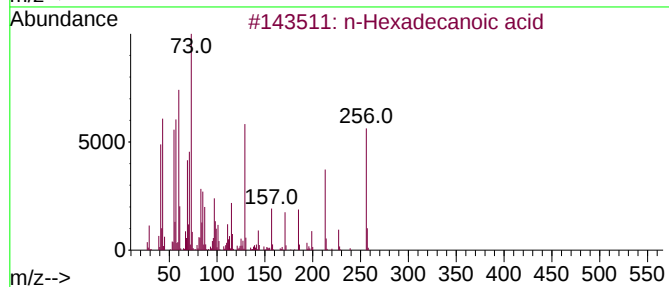
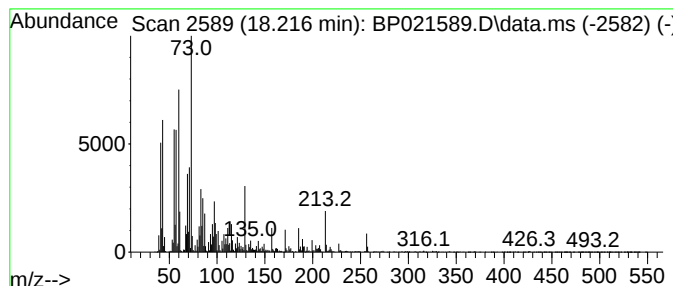
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.216	5.64 ng	1463670	Phenanthrene-d10	17.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Octadecanoic acid	284	C18H36O2	000057-11-4	87
3			Dodecanoic acid	200	C12H24O2	000143-07-7	64
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	62
5			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	53



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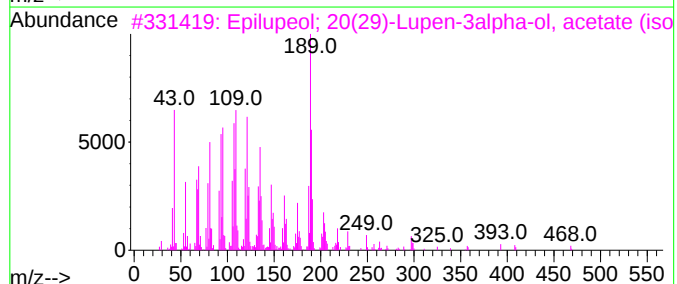
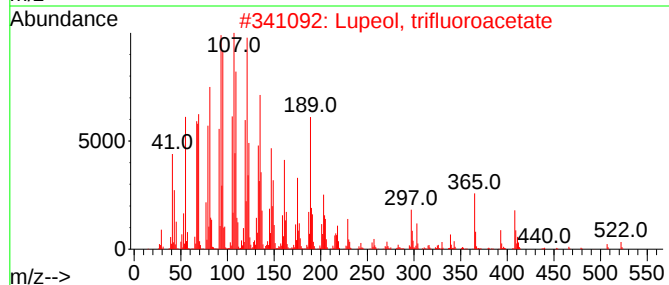
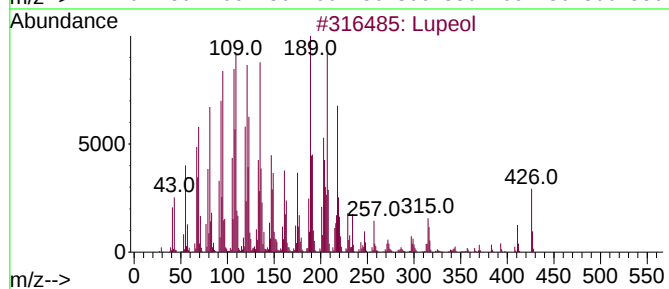
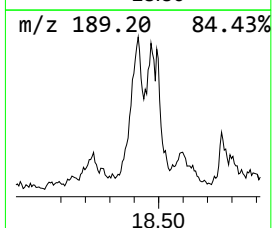
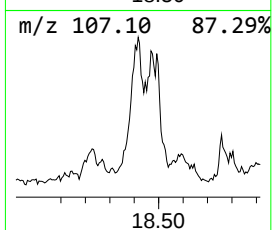
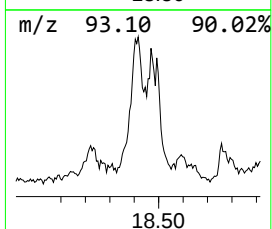
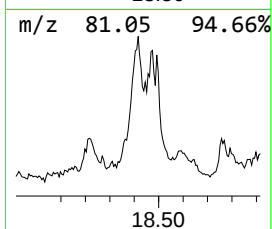
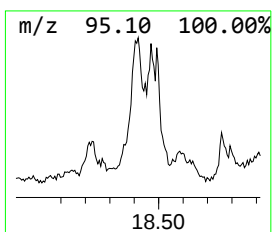
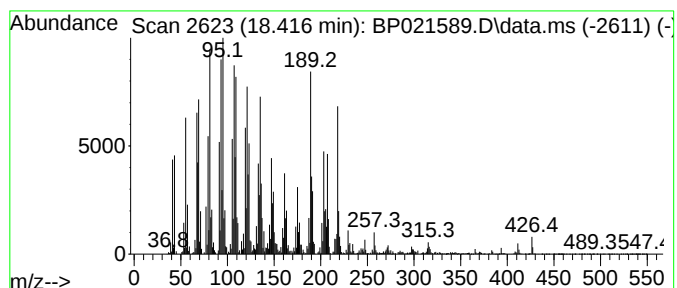
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Peak Number 4 Lupeol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.416	10.67 ng	2771660	Phenanthrene-d10	17.269	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lupeol	426	C30H50O	000545-47-1	98
2	Lupeol, trifluoroacetate	522	C32H49F3O2	1000394-56-7	76
3	Epilupeol; 20(29)-Lupen-3alpha-o...	468	C32H52O2	1010513-01-8	64
4	Epilupeol; 20(29)-Lupen-3alpha-o...	426	C30H50O	1000513-01-3	64
5	Epilupeol; 20(29)-Lupen-3alpha-o...	426	C30H50O	1000513-01-4	56



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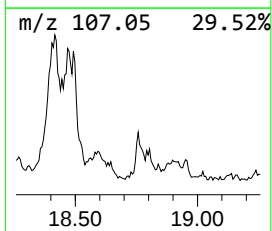
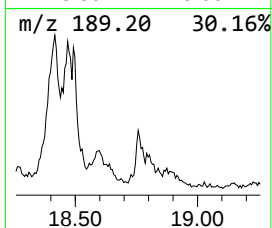
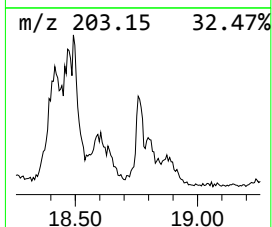
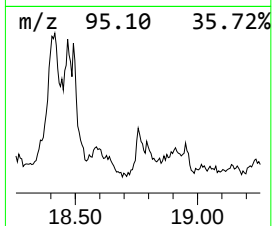
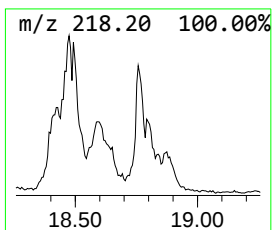
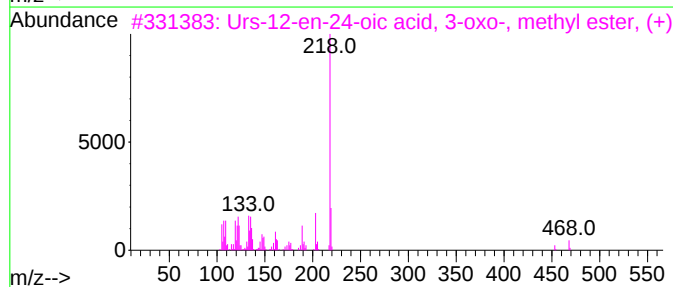
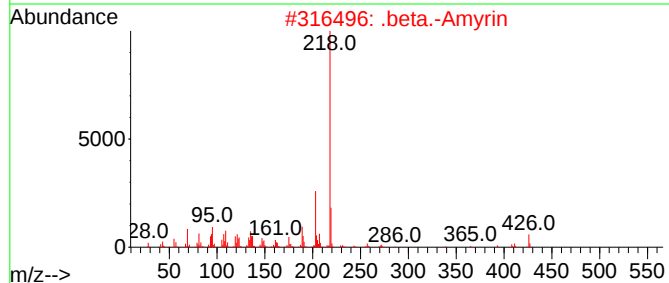
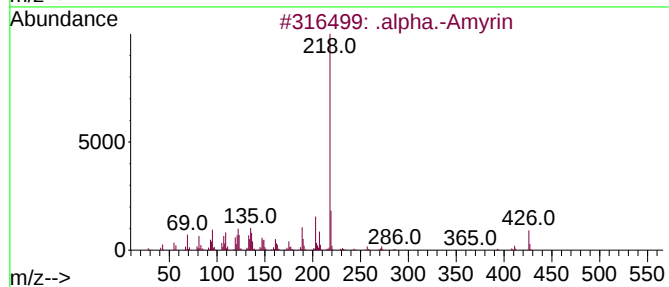
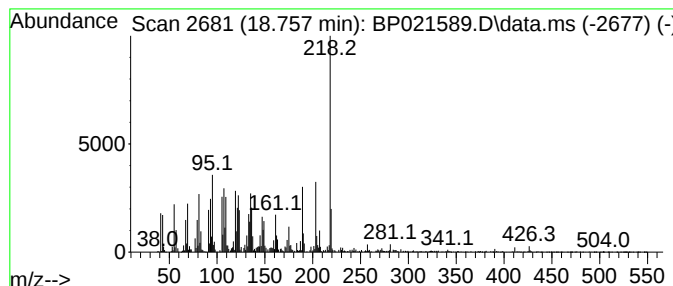
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Peak Number 5 .alpha.-Amyrin Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.757	2.53 ng	657456	Phenanthrene-d10	17.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.alpha.-Amyrin	426	C30H50O	000638-95-9	96
2			.beta.-Amyrin	426	C30H50O	000559-70-6	93
3			Urs-12-en-24-oic acid, 3-oxo-, m...	468	C31H48O3	020475-86-9	86
4			Urs-12-en-3-ol, acetate, (3.beta.)-	468	C32H52O2	000863-76-3	68
5			5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218	C15H22O	006754-66-1	49



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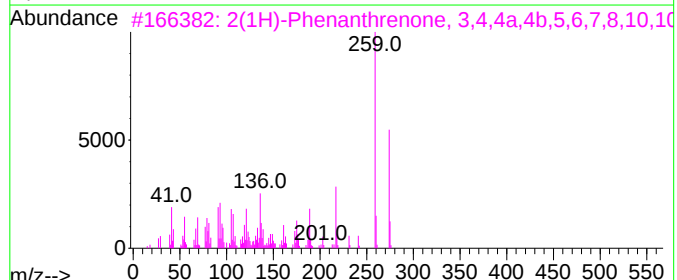
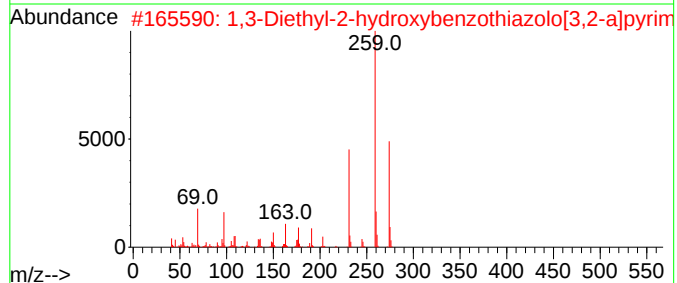
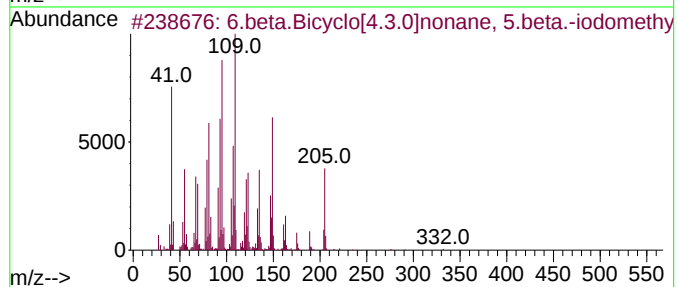
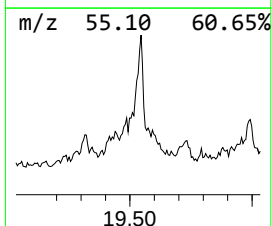
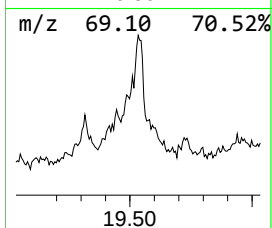
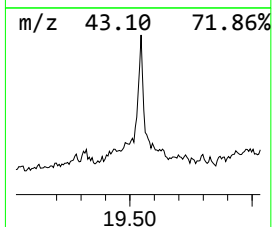
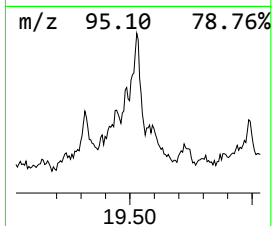
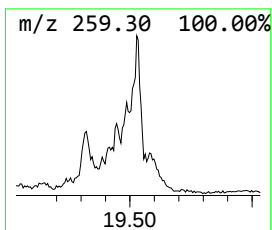
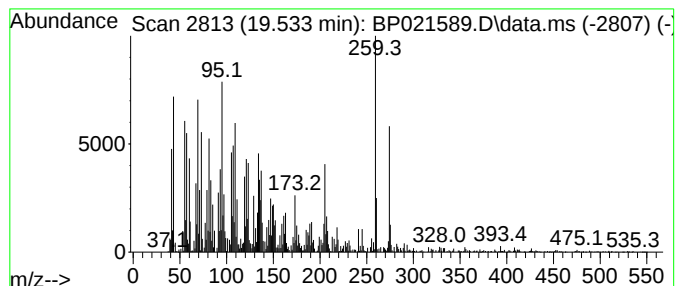
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown19.534 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.534	4.16 ng	1145350	Chrysene-d12	21.727

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6.beta.Bicyclo[4.3.0]nonane, 5.b...			332	C15H25I	1000195-85-9	38
2	1,3-Diethyl-2-hydroxybenzothiazo...			274	C14H14N2O2S	1000227-15-3	35
3	2(1H)-Phenanthrenone, 3,4,4a,4b,...			274	C19H30O	007715-44-8	35
4	Lupeol			426	C30H50O	000545-47-1	30
5	Glutinol			426	C30H50O	000545-24-4	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082024\
Data File : BP021589.D
Acq On : 21 Aug 2024 02:44
Operator : RC/JU
Sample : P3657-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
917-J-WS-081624

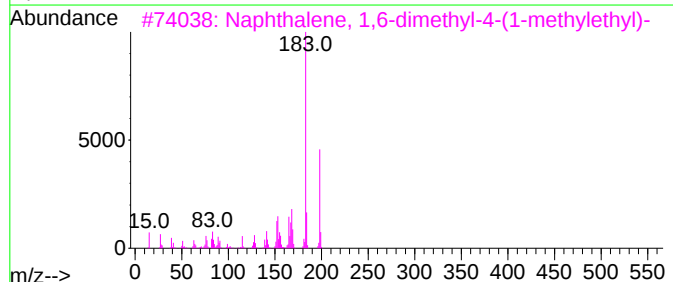
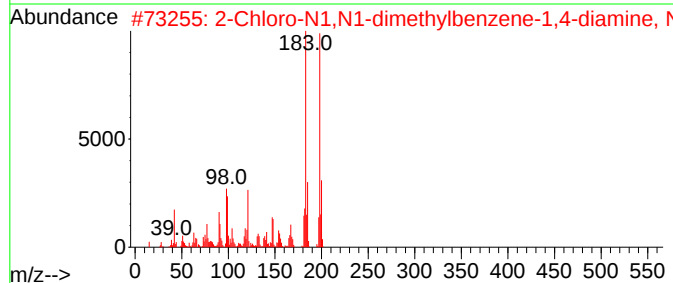
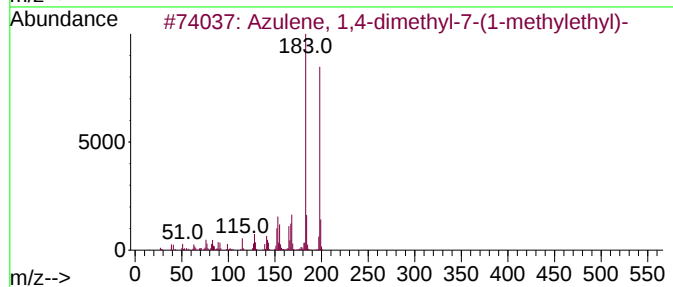
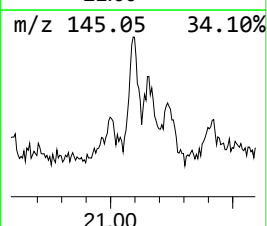
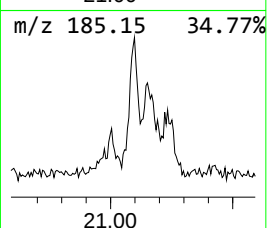
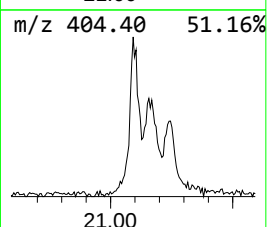
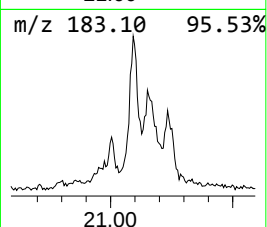
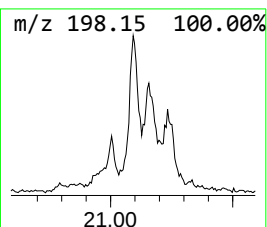
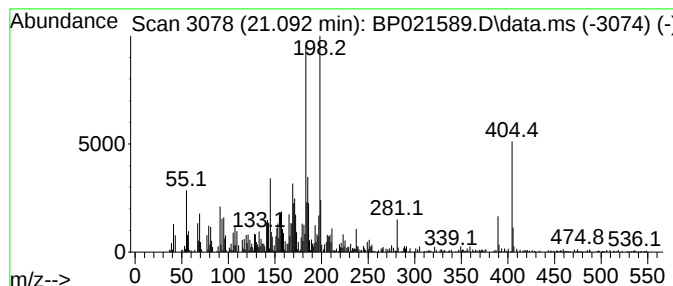
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Azulene, 1,4-dimethyl-7-(1-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.092	2.36 ng	650204	Chrysene-d12	21.727

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azulene, 1,4-dimethyl-7-(1-methy...	198	C15H18	000489-84-9	55
2			2-Chloro-N1,N1-dimethylbenzene-1...	198	C10H15ClN2	1000509-37-8	46
3			Naphthalene, 1,6-dimethyl-4-(1-m...	198	C15H18	000483-78-3	46
4			1,2,3,4-Tetrahydrophenanthrene-4...	198	C14H14O	056179-82-9	35
5			Pyrrolo[1,2-a]pyrazine-1,4-dione...	349	C21H23N3O2	041222-64-4	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082024\
Data File : BP021589.D
Acq On : 21 Aug 2024 02:44
Operator : RC/JU
Sample : P3657-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
917-J-WS-081624

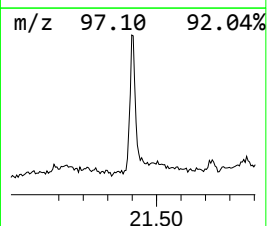
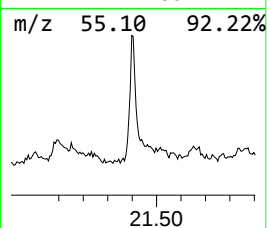
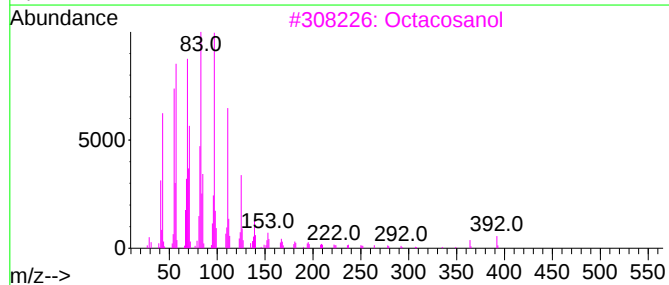
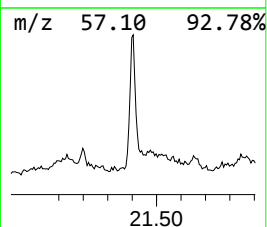
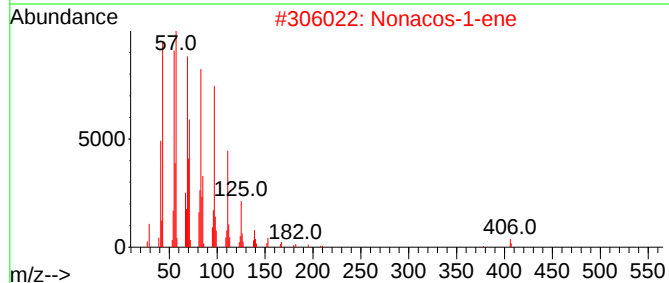
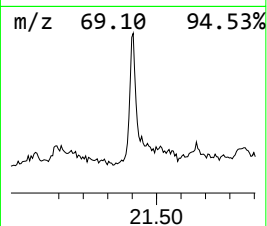
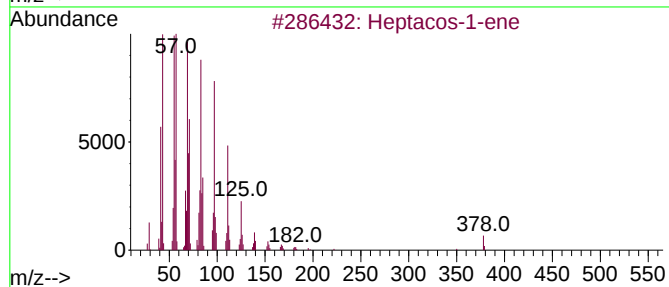
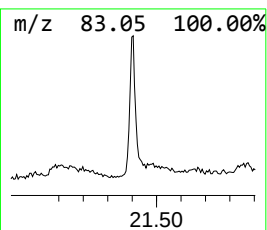
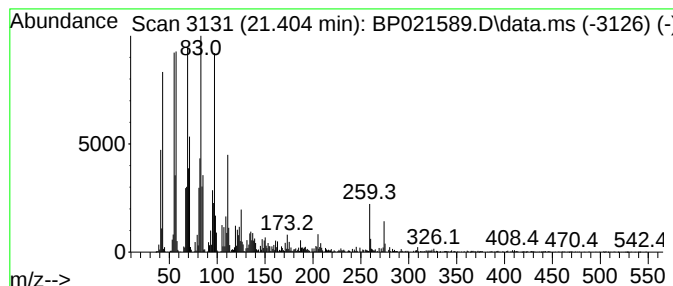
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacos-1-ene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.404	5.44 ng	1496690	Chrysene-d12	21.727

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacos-1-ene	378	C27H54	015306-27-1	91
2			Nonacos-1-ene	406	C29H58	018835-35-3	91
3			Octacosanol	410	C28H58O	000557-61-9	87
4			Eicosyl methyl ether	312	C21H44O	1000406-29-4	87
5			n-Nonadecanol-1	284	C19H40O	001454-84-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082024\
Data File : BP021589.D
Acq On : 21 Aug 2024 02:44
Operator : RC/JU
Sample : P3657-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
917-J-WS-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.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...	3.028	124.1	ng	13090400	1	7.805	2109650	20.0
1-Phenoxypropan...	11.334	2.4	ng	363595	2	10.599	3089590	20.0
n-Hexadecanoic ...	18.216	5.6	ng	1463670	4	17.269	5194150	20.0
Lupeol	18.416	10.7	ng	2771660	4	17.269	5194150	20.0
.alpha.-Amyrin	18.757	2.5	ng	657456	4	17.269	5194150	20.0
unknown19.534	19.534	4.2	ng	1145350	5	21.727	5504100	20.0
Azulene, 1,4-di...	21.092	2.4	ng	650204	5	21.727	5504100	20.0
Heptacos-1-ene	21.404	5.4	ng	1496690	5	21.727	5504100	20.0