

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
 Data File : BM028476.D
 Acq On : 20 Jan 2021 20:08
 Operator : CG/JU
 Sample : M1160-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SP-1

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_M\Methods\8270-BM012021.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM028476.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.075	314	321	329	rBV	26612	39050	3.80%	0.469%
2	5.557	396	403	410	rBV	506867	752075	73.27%	9.039%
3	6.681	589	594	599	rBV	8274	11671	1.14%	0.140%
4	7.193	672	681	691	rBV	484945	776151	75.62%	9.328%
5	7.628	751	755	764	rBV	6440	10484	1.02%	0.126%
6	8.034	818	824	830	rVB	127996	201271	19.61%	2.419%
7	8.804	950	955	961	rVB	8483	12442	1.21%	0.150%
8	9.204	1015	1023	1031	rBV	305566	496062	48.33%	5.962%
9	10.845	1295	1302	1310	rBV	161274	262993	25.62%	3.161%
10	12.298	1544	1549	1553	rBV2	14695	20645	2.01%	0.248%
11	13.298	1712	1719	1729	rVB	624669	922357	89.86%	11.085%
12	14.074	1846	1851	1855	rBV	8063	10643	1.04%	0.128%
13	14.121	1855	1859	1866	rVB	31747	41528	4.05%	0.499%
14	14.504	1914	1924	1929	rBV4	11441	21368	2.08%	0.257%
15	14.621	1939	1944	1947	rBV	20794	26902	2.62%	0.323%
16	14.669	1947	1952	1959	rVV	211800	302866	29.51%	3.640%
17	14.727	1959	1962	1972	rVB2	11177	16737	1.63%	0.201%
18	14.916	1989	1994	1999	rVB	21038	26844	2.62%	0.323%
19	14.980	2001	2005	2009	rBV3	7422	11449	1.12%	0.138%
20	16.151	2192	2204	2211	rBV	489696	696677	67.88%	8.373%
21	16.221	2211	2216	2221	rVB3	14306	21551	2.10%	0.259%
22	17.398	2410	2416	2424	rBV	238049	340359	33.16%	4.091%
23	17.762	2472	2478	2484	rBV4	14025	25312	2.47%	0.304%
24	18.209	2550	2554	2559	rBV2	9758	15093	1.47%	0.181%
25	18.268	2559	2564	2576	rBV	110943	169054	16.47%	2.032%
26	19.121	2705	2709	2715	rBV5	7392	12872	1.25%	0.155%
27	19.421	2756	2760	2767	rBV3	18050	32062	3.12%	0.385%
28	19.533	2776	2779	2786	rBV3	18696	26729	2.60%	0.321%
29	19.898	2837	2841	2844	rVB	19682	23057	2.25%	0.277%
30	19.986	2851	2856	2861	rBV	818714	1026389	100.00%	12.335%
31	20.250	2899	2901	2904	rBV3	10276	11591	1.13%	0.139%
32	20.615	2959	2963	2967	rBV	16455	21447	2.09%	0.258%
33	21.074	3037	3041	3046	rBV	82653	98984	9.64%	1.190%
34	21.227	3062	3067	3075	rBV	152524	201969	19.68%	2.427%
35	21.527	3113	3118	3127	rBV	293062	373640	36.40%	4.490%
36	22.121	3216	3219	3227	rVB	79179	109041	10.62%	1.310%

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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 >
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37	23.086	3379	3383	3388	rBV	110294	157011	15.30%	1.887%
38	23.139	3388	3392	3400	rVB2	56663	95821	9.34%	1.152%
39	23.815	3501	3507	3515	rVB2	184785	356036	34.69%	4.279%
40	24.109	3552	3557	3568	rVB	175075	351393	34.24%	4.223%
41	24.333	3590	3595	3604	rVB	100526	191064	18.62%	2.296%

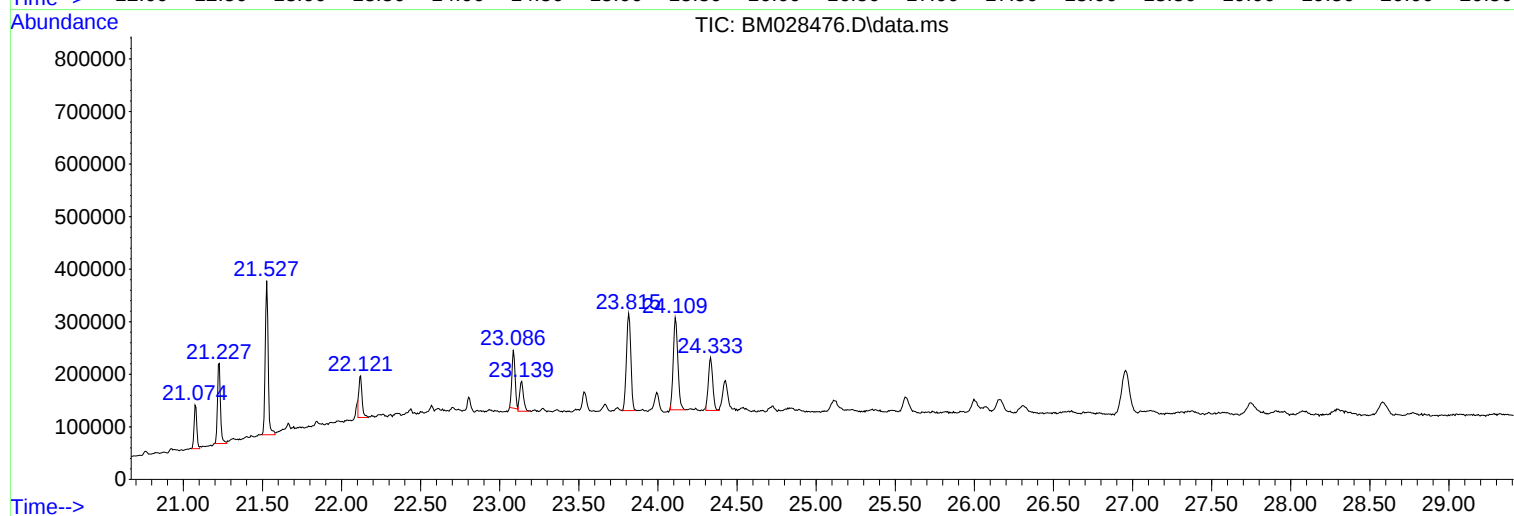
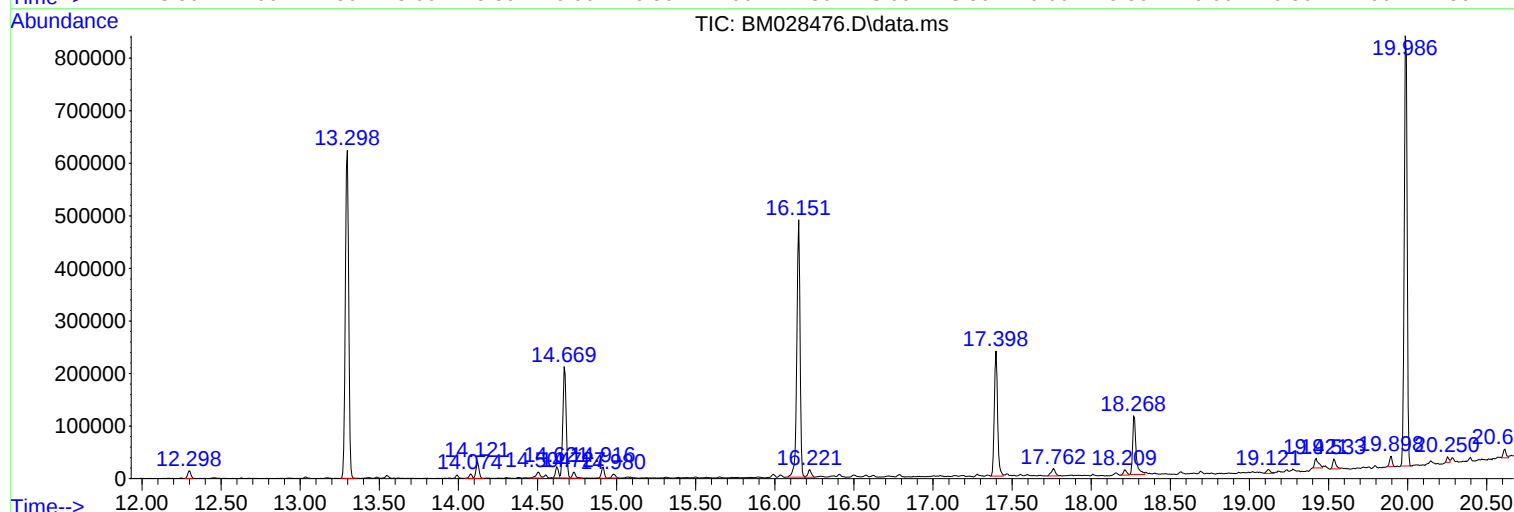
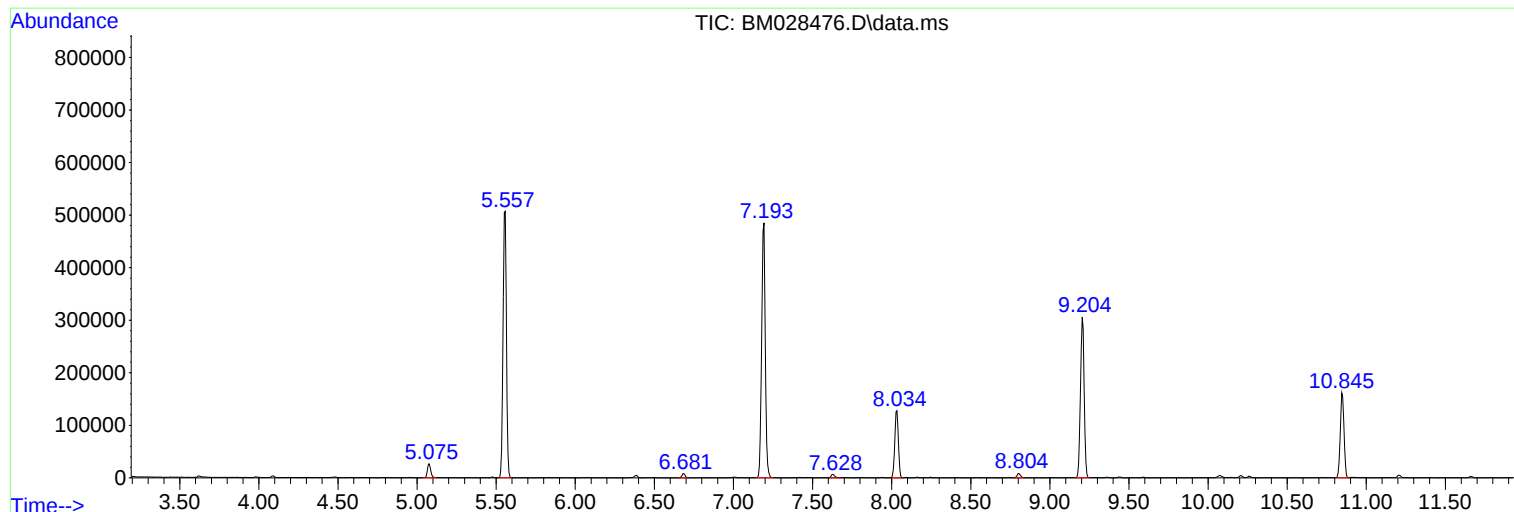
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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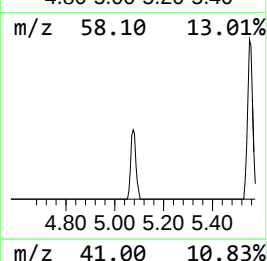
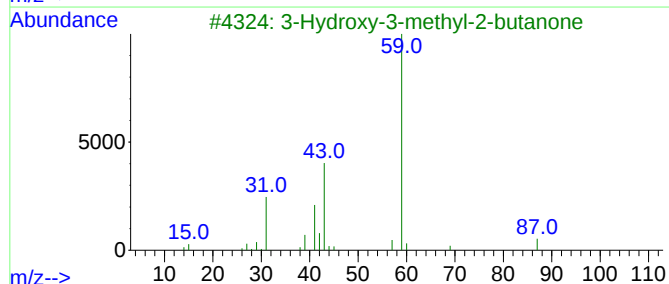
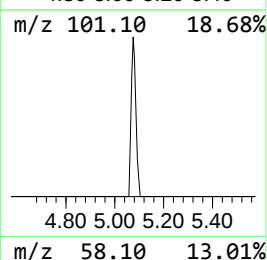
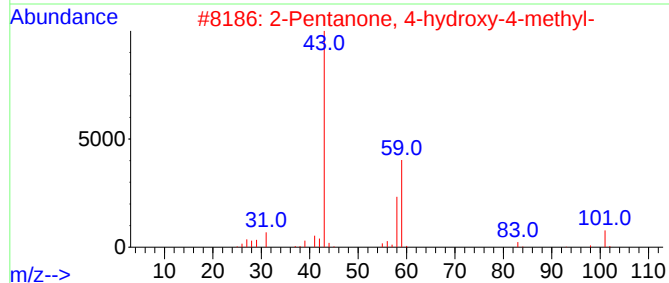
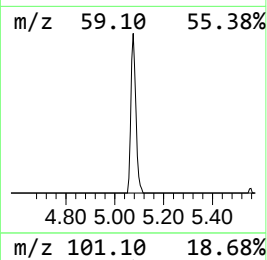
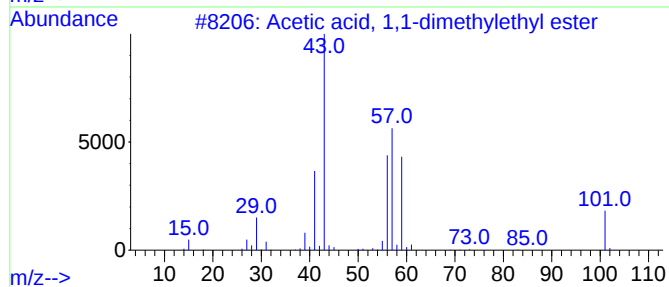
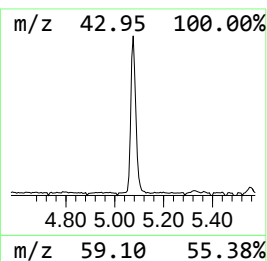
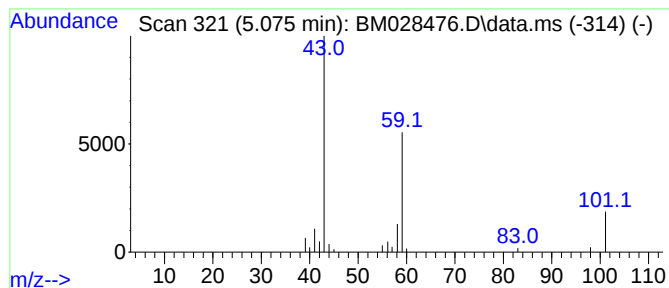
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown5.075 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	3.88 ng	39050	1,4-Dichlorobenzene-d4	8.034

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
3		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23
4		Diacetamide	101	C4H7NO2	000625-77-4	9
5		Propylamine	59	C3H9N	000107-10-8	9



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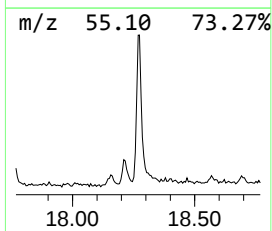
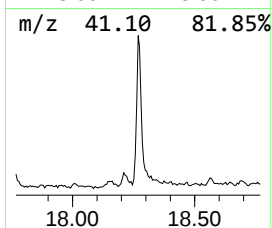
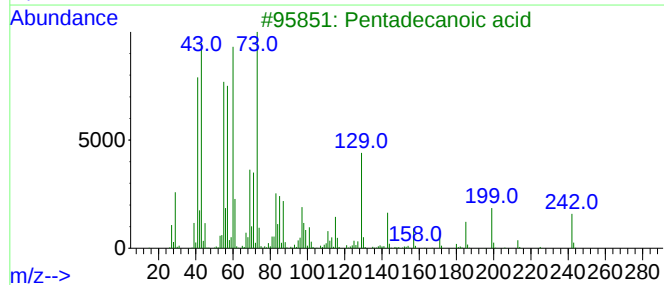
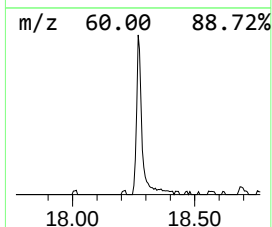
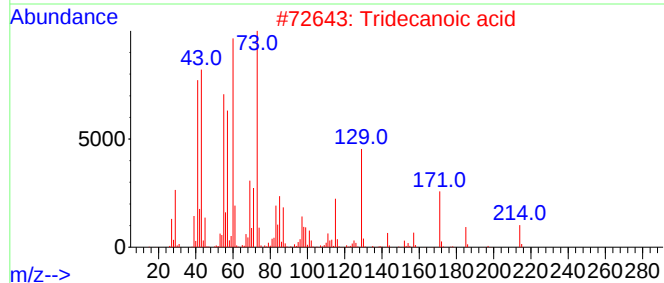
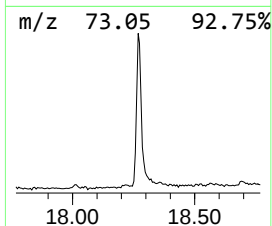
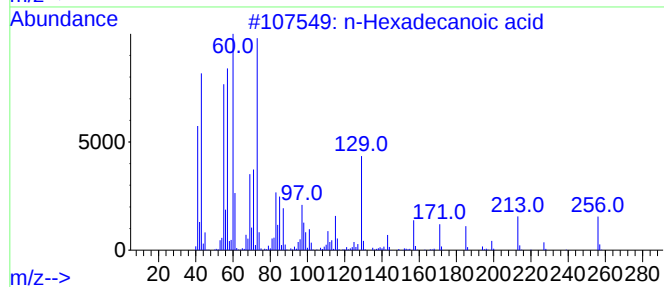
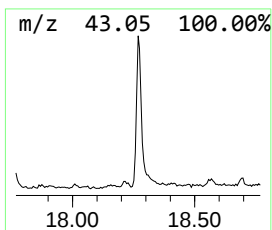
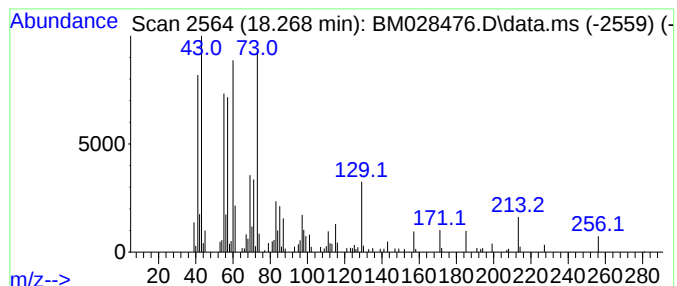
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.268	9.93 ng	169054	Phenanthrene-d10	17.398

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	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	72



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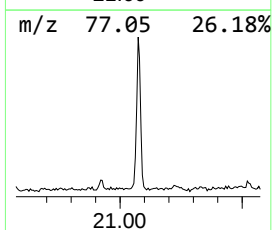
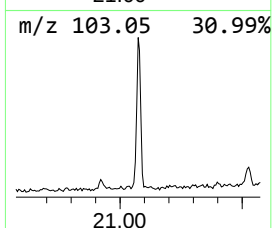
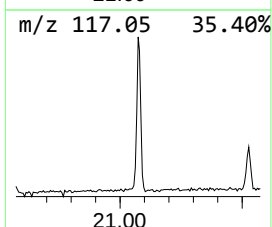
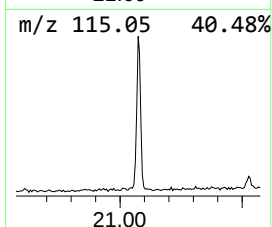
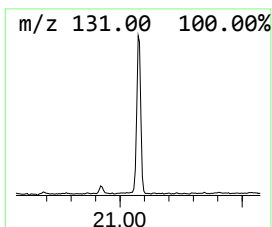
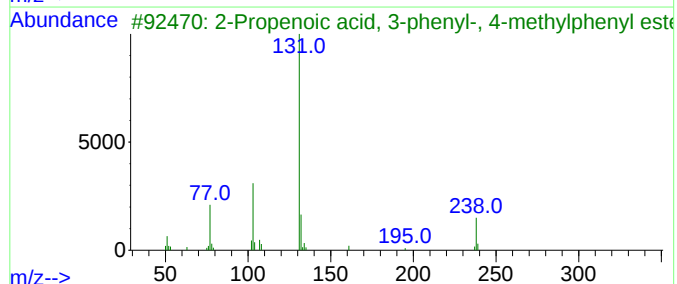
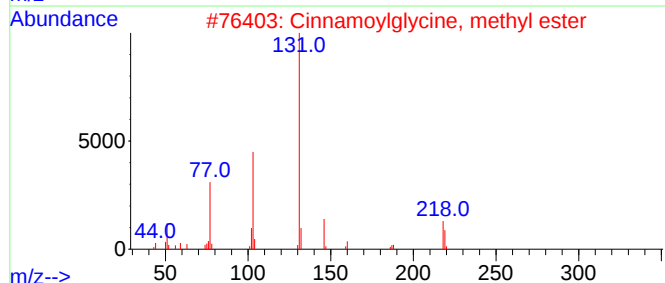
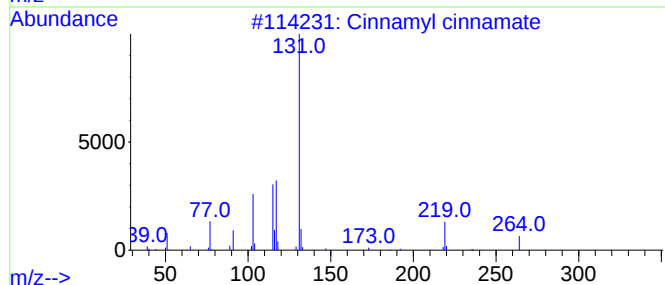
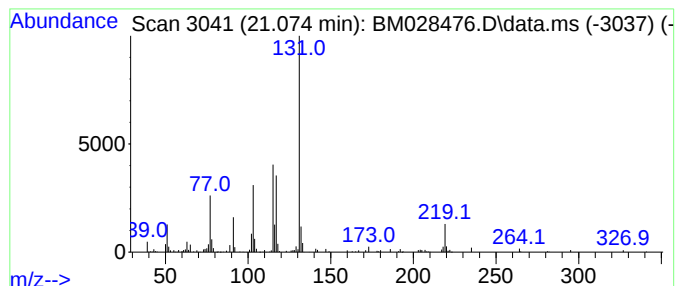
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Cinnamyl cinnamate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.074	5.30 ng	98984	Chrysene-d12	21.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	87
2			Cinnamoylglycine, methyl ester	219	C12H13NO3	040778-04-9	83
3			2-Propenoic acid, 3-phenyl-, 4-m...	238	C16H14O2	010519-07-0	47
4			2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	47
5			2,4,5-Trichlorophenyl cinnamate	326	C15H9Cl3O2	1000242-39-6	47



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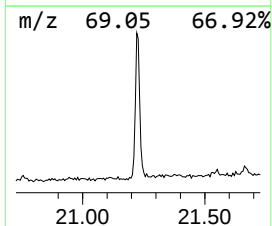
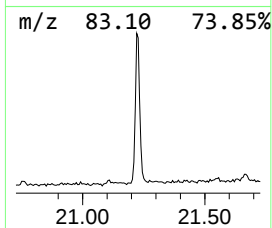
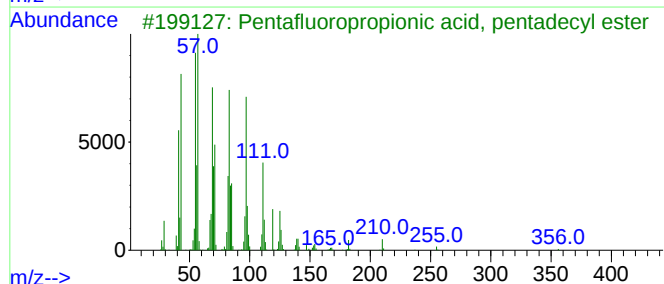
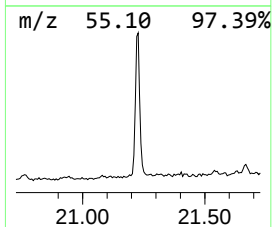
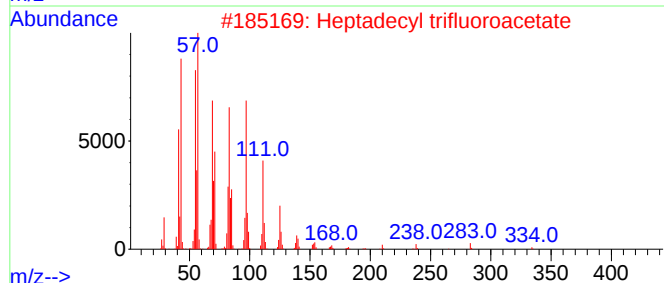
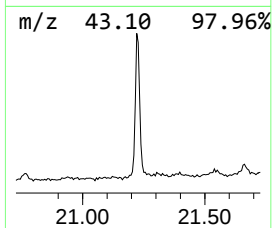
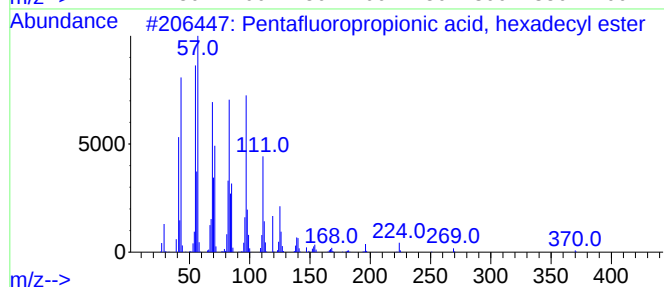
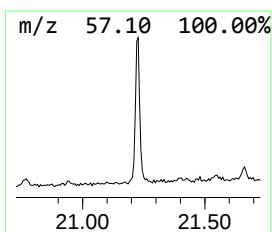
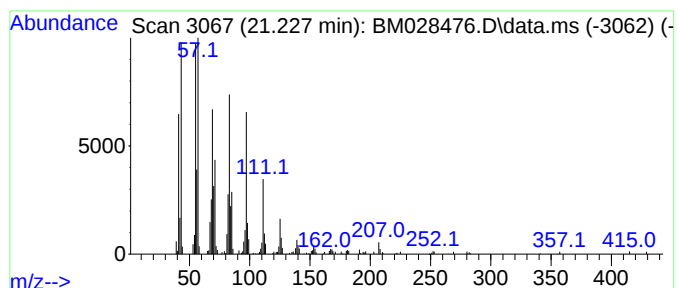
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Pentafluoropropionic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.227	10.81 ng	201969	Chrysene-d12	21.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
3			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94



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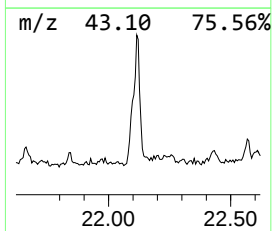
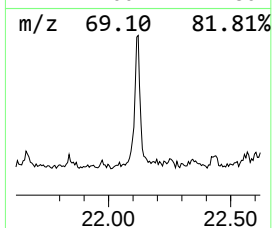
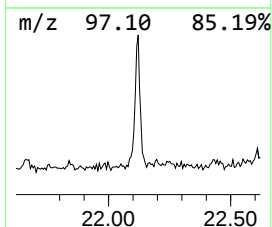
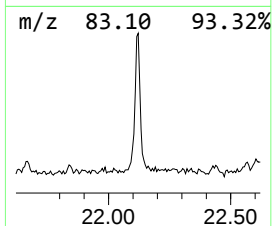
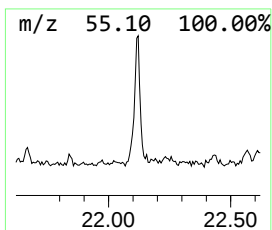
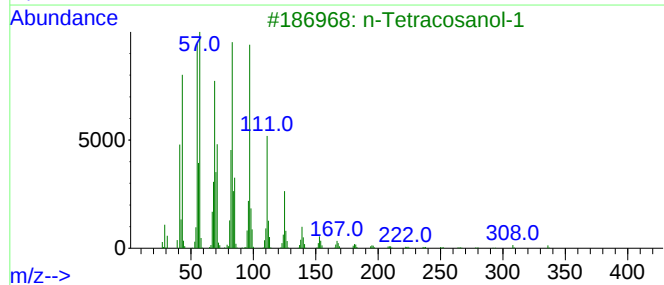
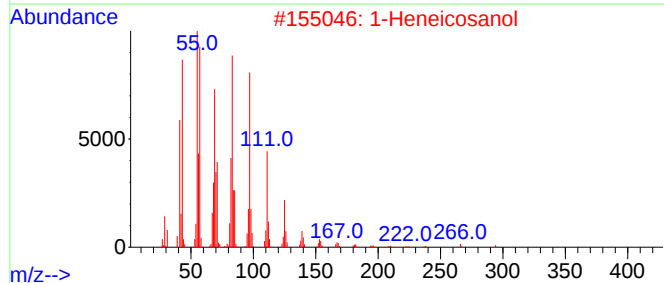
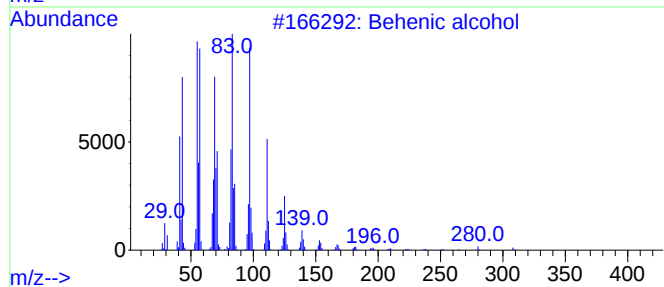
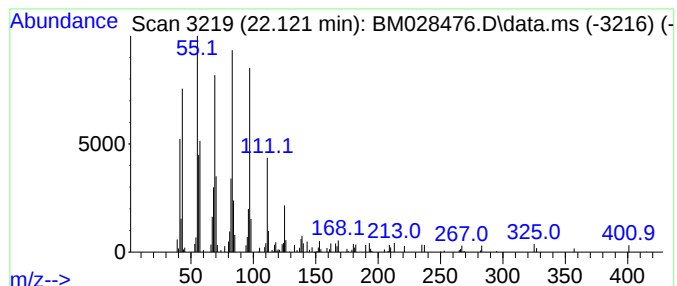
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.121	5.84 ng	109041	Chrysene-d12	21.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	90
2			1-Heneicosanol	312	C21H44O	015594-90-8	90
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	87
4			1-Heptacosanol	396	C27H56O	002004-39-9	68
5			Cyclooctacosane	392	C28H56	000297-24-5	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028476.D
Acq On : 20 Jan 2021 20:08
Operator : CG/JU
Sample : M1160-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-1

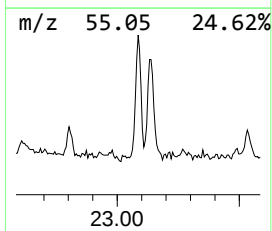
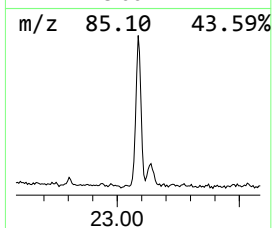
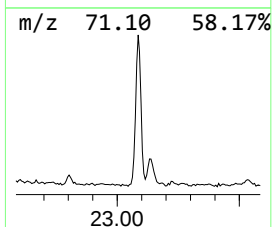
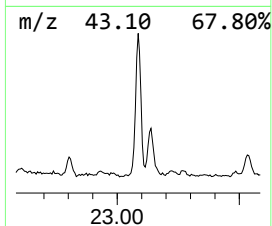
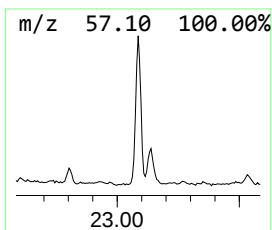
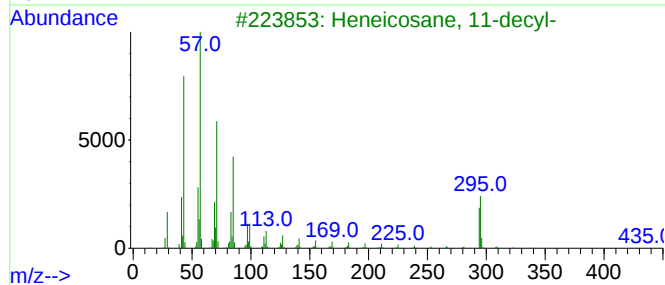
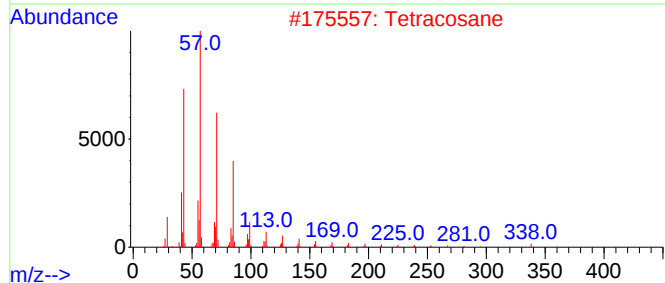
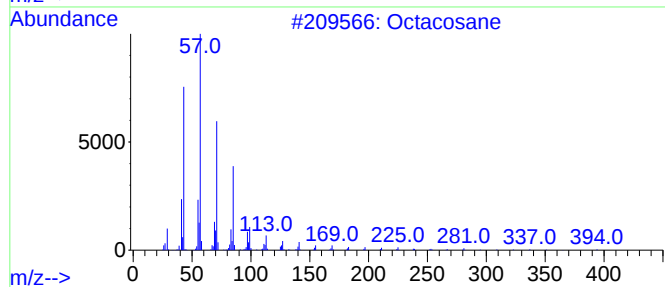
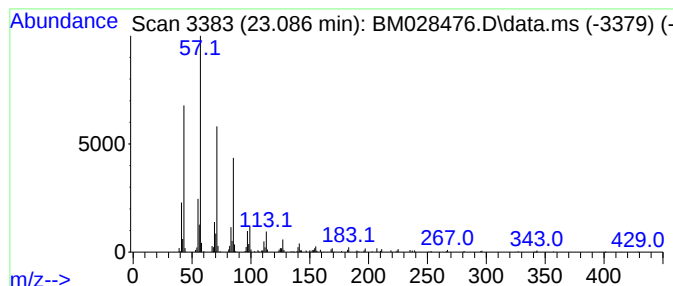
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.086	8.82 ng	157011	Perylene-d12	23.815

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	91
2		Tetracosane	338	C24H50	000646-31-1	91
3		Heneicosane, 11-decyl-	437	C31H64	055320-06-4	91
4		Docosane, 7-hexyl-	394	C28H58	055373-86-9	91
5		Eicosane, 9-octyl-	394	C28H58	013475-77-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
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Acq On : 20 Jan 2021 20:08
Operator : CG/JU
Sample : M1160-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

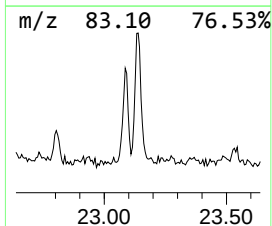
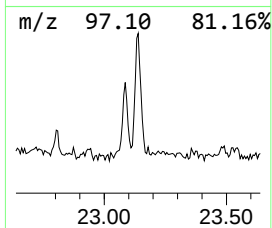
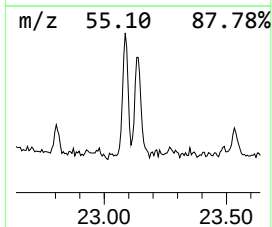
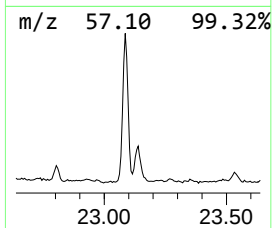
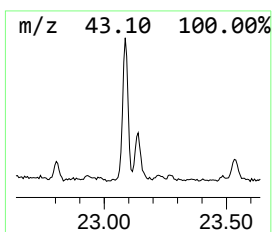
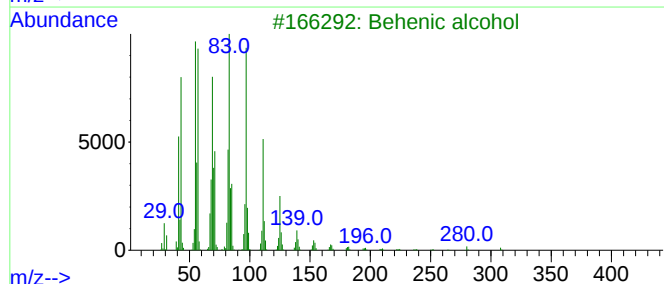
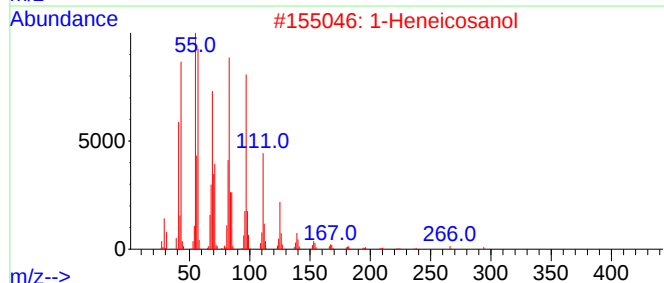
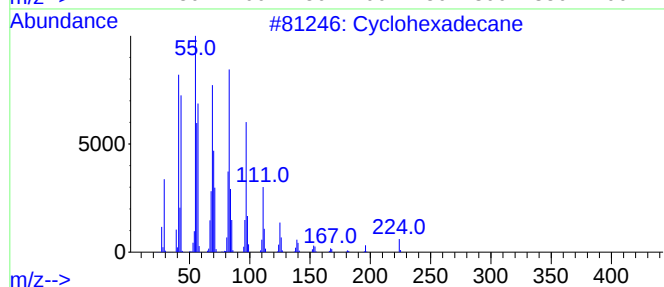
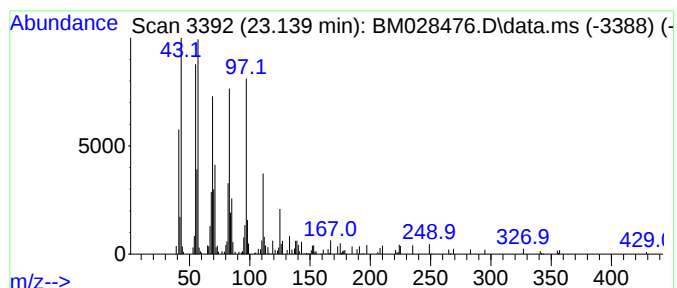
Instrument :
BNA_M
ClientSampled :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclohexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.139	5.38 ng	95821	Perylene-d12	23.815	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	96
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028476.D
Acq On : 20 Jan 2021 20:08
Operator : CG/JU
Sample : M1160-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-1

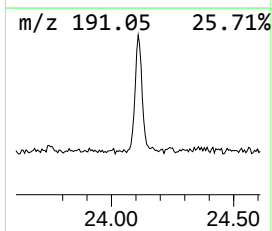
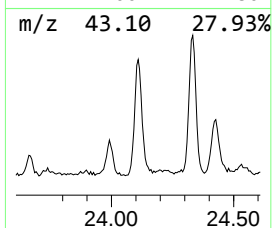
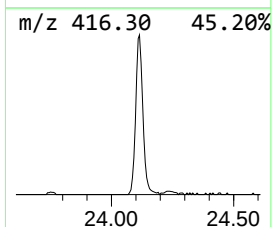
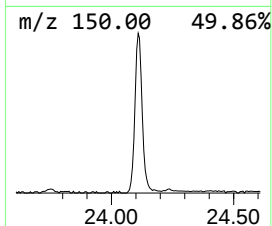
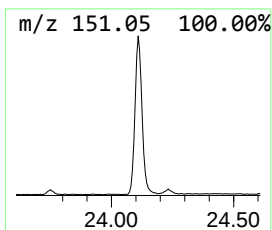
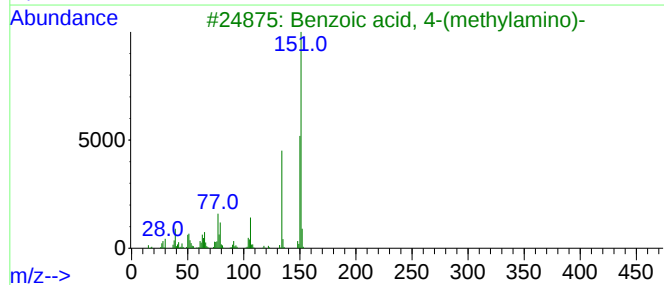
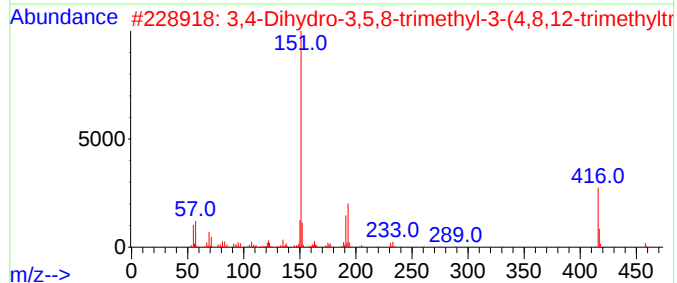
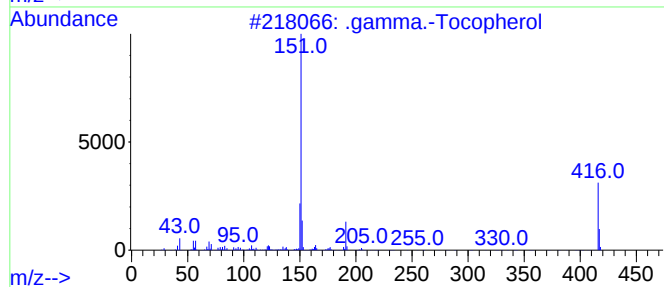
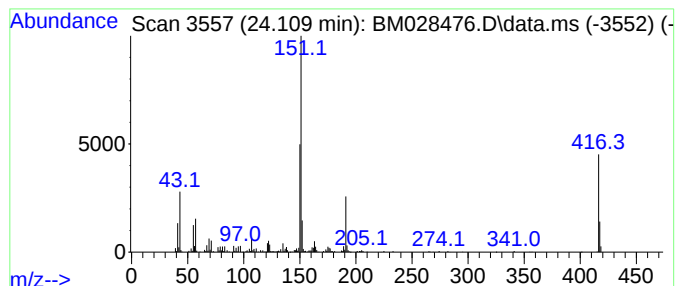
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 .gamma.-Tocopherol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.109	19.74 ng	351393	Perylene-d12	23.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.gamma.-Tocopherol	416	C28H48O2	007616-22-0	95
2			3,4-Dihydro-3,5,8-trimethyl-3-(4...	458	C30H50O3	1000105-71-9	53
3			Benzoic acid, 4-(methylamino)-	151	C8H9NO2	010541-83-0	47
4			4-Ethylbenzoic acid, octadecyl e...	402	C27H46O2	1000292-35-1	38
5			3,4-Dimethoxy-dl-phenylalanine	225	C11H15NO4	033522-62-2	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028476.D
Acq On : 20 Jan 2021 20:08
Operator : CG/JU
Sample : M1160-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-1

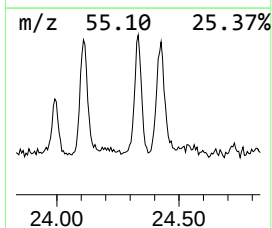
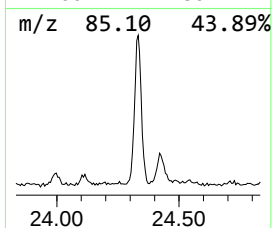
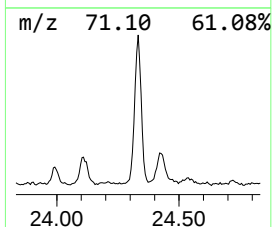
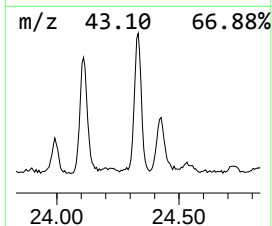
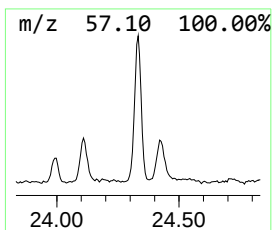
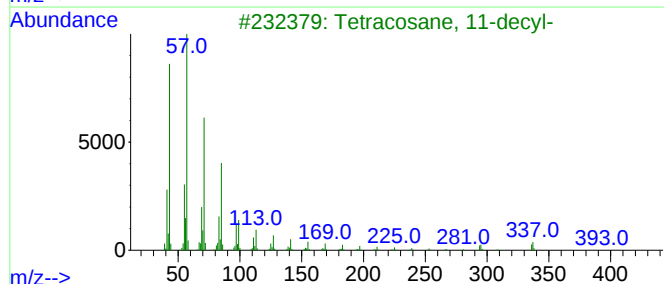
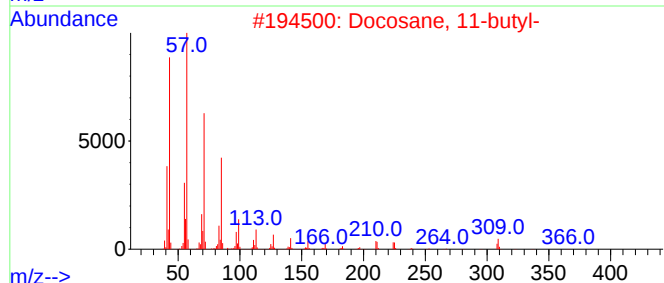
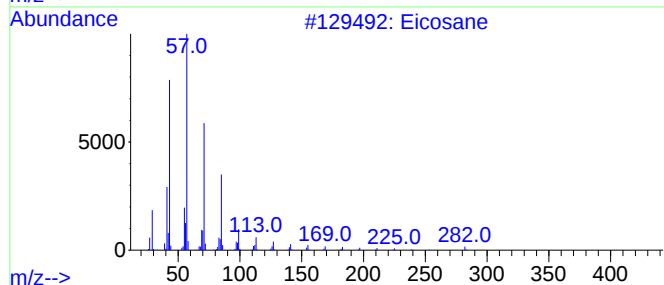
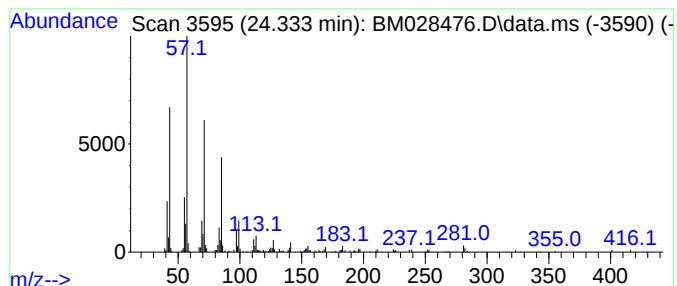
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.333	10.73 ng	191064	Perylene-d12	23.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	98
2			Docosane, 11-butyl-	366	C26H54	013475-76-8	90
3			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	90
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5			Tetracosane	338	C24H50	000646-31-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
 Data File : BM028476.D
 Acq On : 20 Jan 2021 20:08
 Operator : CG/JU
 Sample : M1160-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.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
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n-Hexadecanoic ...	18.268	9.9	ng	169054	4	17.398	340359	20.0
Cinnamyl cinnamate	21.074	5.3	ng	98984	5	21.527	373640	20.0
Pentafluoroprop...	21.227	10.8	ng	201969	5	21.527	373640	20.0
Behenic alcohol	22.121	5.8	ng	109041	5	21.527	373640	20.0
Octacosane	23.086	8.8	ng	157011	6	23.815	356036	20.0
Cyclohexadecane	23.139	5.4	ng	95821	6	23.815	356036	20.0
.gamma.-Tocopherol	24.109	19.7	ng	351393	6	23.815	356036	20.0
Eicosane	24.333	10.7	ng	191064	6	23.815	356036	20.0