LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040821\
Data File : BP005239.D
Acq On : 08 Apr 2021 16:59
Operator : CG/JU
Sample : M1973-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BU-02-040721

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-BP032321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005239.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.287	368	374	382	rVB	528371	738140	41.84%	7.209%
2	6.369	553	558	566	rVB2	48028	72767	4.12%	0.711%
3	6.869	636	643	653	rVB	445136	708656	40.17%	6.921%
4	7.581	759	764	770	rVB2	18549	28403	1.61%	0.277%
5	7.687	776	782	789	rVB	85524	132698	7.52%	1.296%
6	8.846	972	979	987	rBV	265197	431718	24.47%	4.216%
7	10.475	1248	1256	1264	rBV	100037	168292	9.54%	1.644%
8	11.846	1483	1489	1496	rBV	28771	44959	2.55%	0.439%
9	12.957	1671	1678	1685	rBV	624405	925171	52.44%	9.036%
10	13.804	1817	1822	1831	rVB	23995	37565	2.13%	0.367%
11	14.346	1908	1914	1921	rBV	150323	215657	12.22%	2.106%
12	15.845	2160	2169	2180	rVB	543243	775731	43.97%	7.576%
13	17.110	2377	2384	2388	rBV	190868	270091	15.31%	2.638%
14	17.151	2388	2391	2397	rVB	28638	41742	2.37%	0.408%
15	18.010	2530	2537	2546	rBV	122362	188812	10.70%	1.844%
16	18.298	2580	2586	2591	rBV7	16965	27158	1.54%	0.265%
17	19.004	2701	2706	2713	rBV9	11026	19071	1.08%	0.186%
18	19.134	2723	2728	2735	rVB	59236	78737	4.46%	0.769%
19	19.251	2743	2748	2757	rBV2	53277	83586	4.74%	0.816%
20	19.486	2784	2788	2797	rVB	35441	58179	3.30%	0.568%
21	19.686	2817	2822	2831	rBV	1502131	1764260	100.00%	17.231%
22	19.969	2866	2870	2876	rVB6	18337	35986	2.04%	0.351%
23	20.316	2925	2929	2931	rBV4	16616	21836	1.24%	0.213%
24	20.345	2931	2934	2935	rVV3	24065	25969	1.47%	0.254%
25	20.363	2935	2937	2943	rVB3	33196	44991	2.55%	0.439%
26	20.569	2968	2972	2978	rBV5	24436	32653	1.85%	0.319%
27	20.751	3000	3003	3008	rBV5	13409	20221	1.15%	0.197%
28	20.928	3029	3033	3040	rVB2	158086	228898	12.97%	2.236%
29	20.992	3040	3044	3052	rVB	94671	113812	6.45%	1.112%
30	21.080	3055	3059	3063	rVV	186918	226626	12.85%	2.213%
31	21.122	3063	3066	3071	rVV	379129	413927	23.46%	4.043%
32	21.210	3075	3081	3085	rVV	348131	471734	26.74%	4.607%
33	21.245	3085	3087	3092	rVB	54980	62532	3.54%	0.611%
34	21.304	3093	3097	3102	rVB	102860	125938	7.14%	1.230%
35	21.510	3128	3132	3139	rBV4	66241	123383	6.99%	1.205%
36	21.816	3177	3184	3195	rBV3	133996	273806	15.52%	2.674%

LSC Area Percent Report

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Instrument : BNA_P
ClientSampleId : BU-02-040721

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-BP032321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	22.004	3213	3216	3220	rVB	35140	39846	2.26%	0.389%
38	22.057	3221	3225	3229	rBV2	60461	71934	4.08%	0.703%
39	22.498	3296	3300	3307	rVB2	57492	72717	4.12%	0.710%
40	22.786	3344	3349	3354	rBV2	103375	195829	11.10%	1.913%
41	22.839	3355	3358	3366	rVB2	59632	104934	5.95%	1.025%
42	23.486	3462	3468	3484	rVB2	221847	442548	25.08%	4.322%
43	23.692	3499	3503	3510	rVB5	64635	118357	6.71%	1.156%
44	25.286	3769	3774	3783	rVB3	69732	159012	9.01%	1.553%

Sum of corrected areas: 10238882

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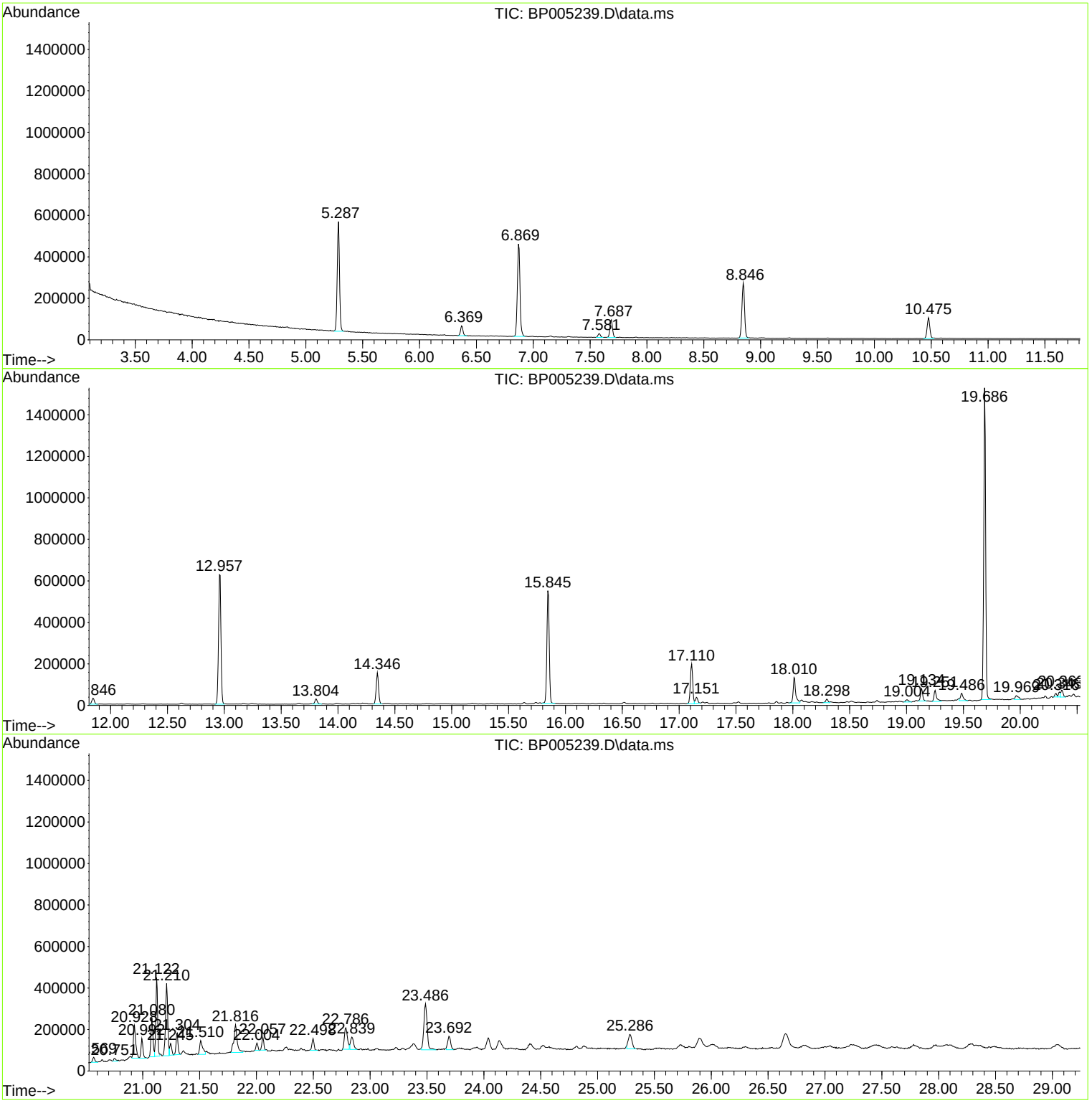
Instrument :
BNA_P
ClientSampleId :
BU-02-040721

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.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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Instrument :
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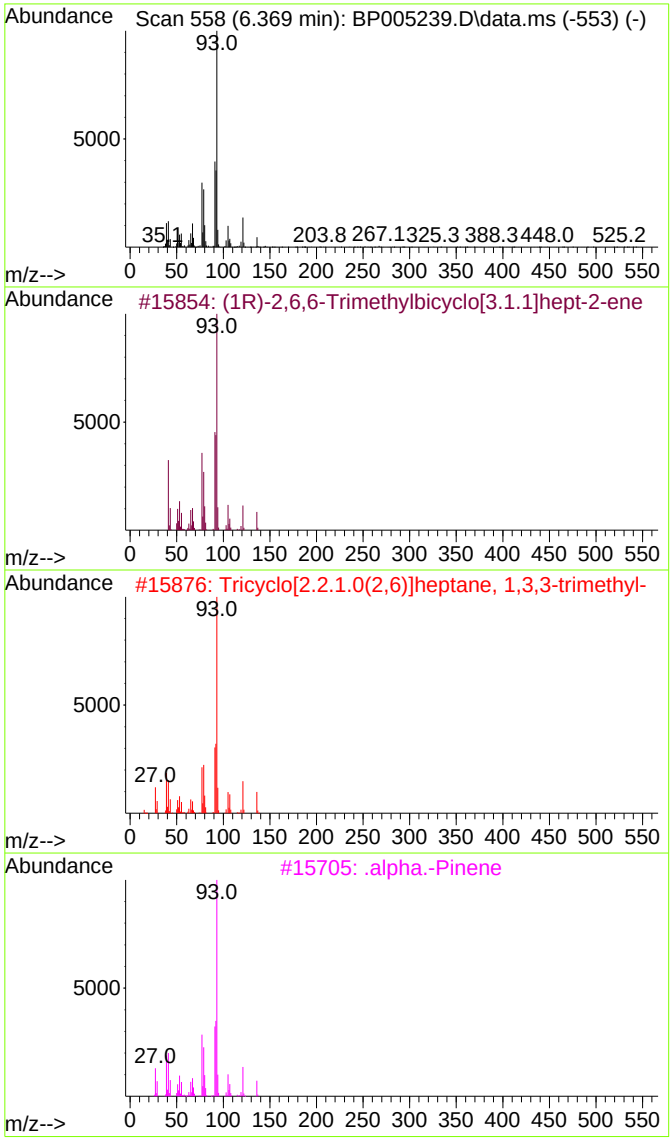
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

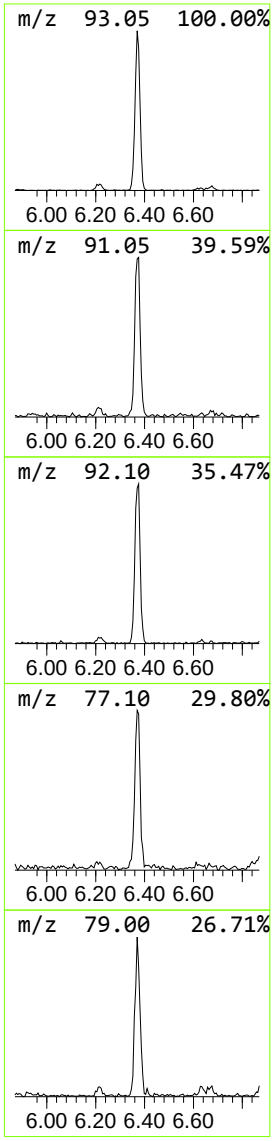
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (1R)-2,6,6-Trimethylbicyclo... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.369	10.97 ng	72767	1,4-Dichlorobenzene-d4	7.687

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	94
2	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	91
3	.alpha.-Pinene	136	C10H16	000080-56-8	91
4	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91
5	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	91





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Data File : BP005239.D
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Operator : CG/JU
Sample : M1973-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BU-02-040721

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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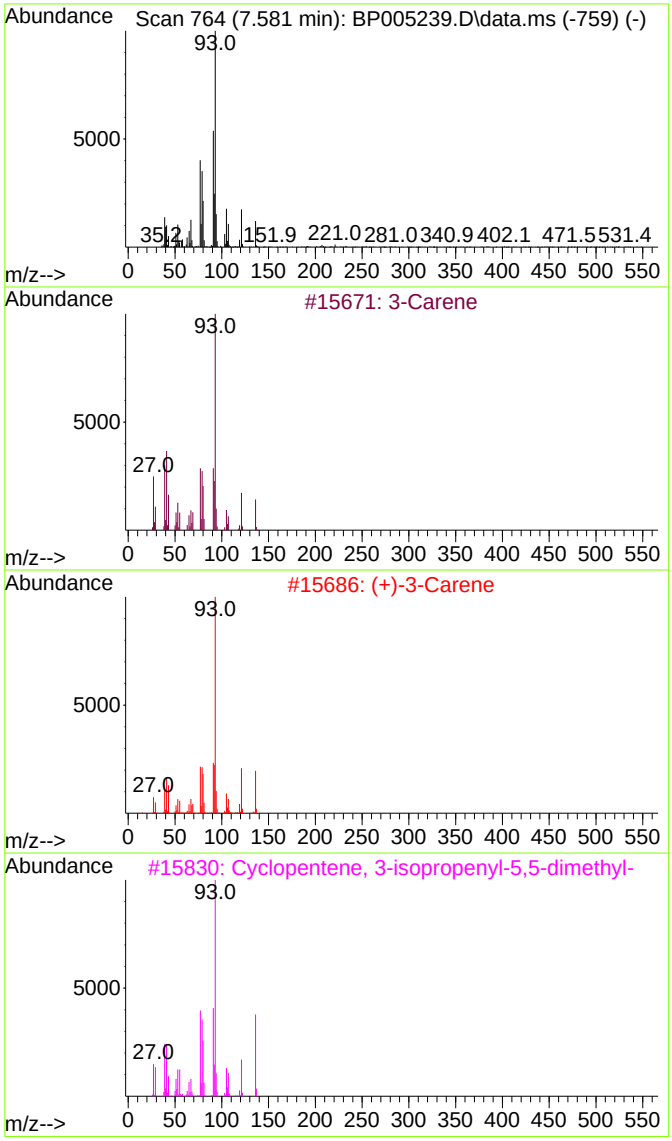
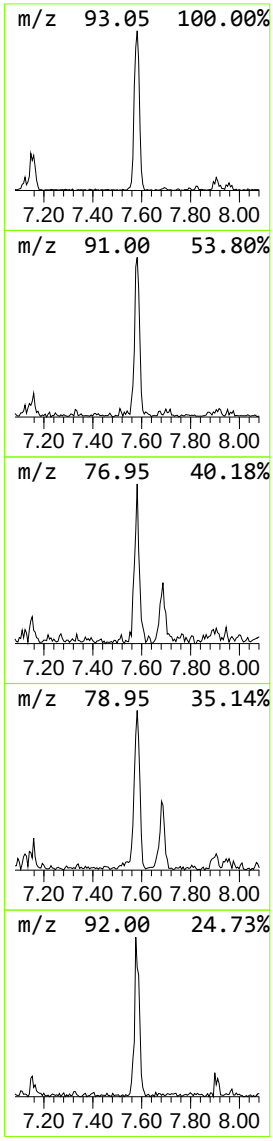
****

Peak Number 2 3-Carene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.581	4.28 ng	28403	1,4-Dichlorobenzene-d4	7.687

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Carene	136	C10H16	013466-78-9	91
2	(+)-3-Carene	136	C10H16	000498-15-7	91
3	Cyclopentene, 3-isopropenyl-5,5-...	136	C10H16	1000162-25-4	90
4	.gamma.-Terpinene	136	C10H16	000099-85-4	90
5	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	90





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Data File : BP005239.D
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Operator : CG/JU
Sample : M1973-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BU-02-040721

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

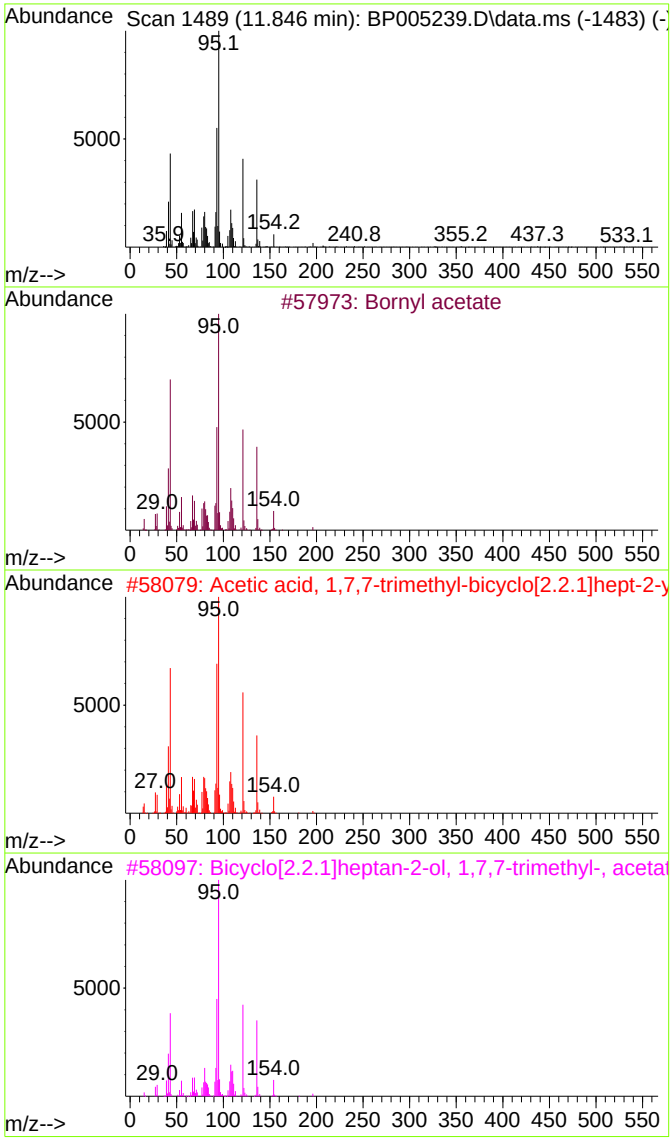
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

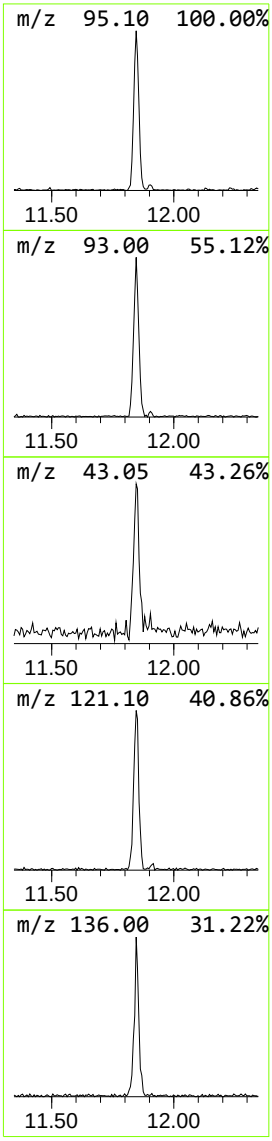
****

Peak Number 3 Bornyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.846	5.34 ng	44959	Naphthalene-d8	10.475

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bornyl acetate	196	C12H20O2	000076-49-3	97
2	Acetic acid, 1,7,7-trimethyl-bic...	196	C12H20O2	092618-89-8	95
3	Bicyclo[2.2.1]heptan-2-ol, 1,7,7...	196	C12H20O2	005655-61-8	91
4	Isobornyl propionate	210	C13H22O2	002756-56-1	80
5	1,2,3,4,4a,5,6,8a-Octahydro-naph...	136	C10H16	031244-58-3	58





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Sample : M1973-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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

TIC Library : C:\DATABASE\NIST11.L
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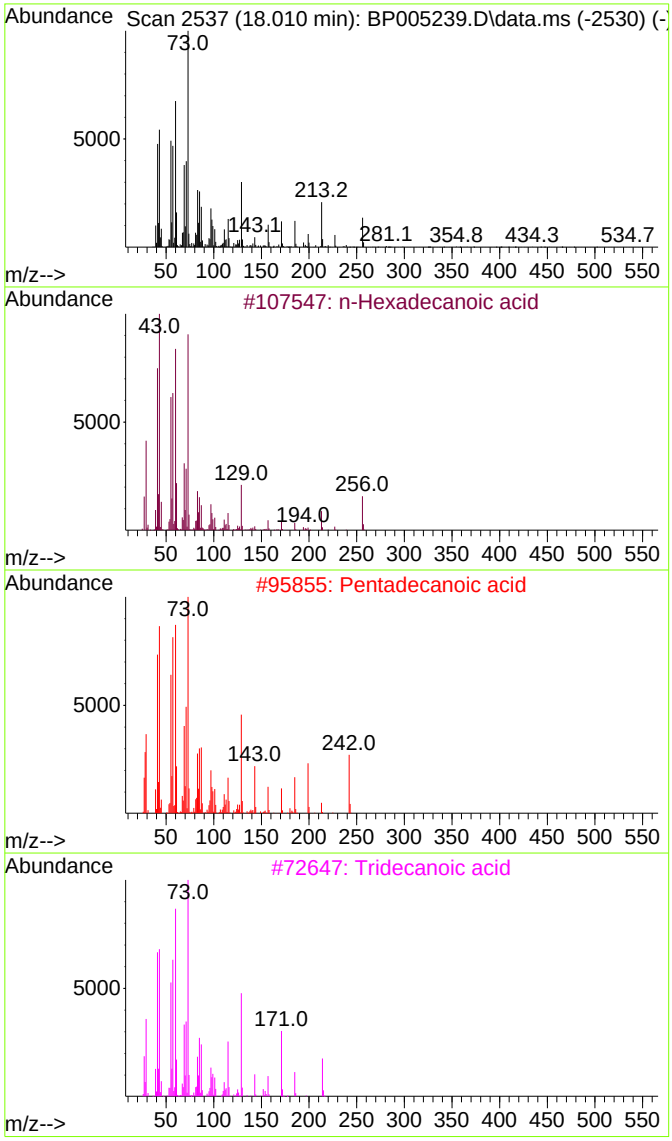
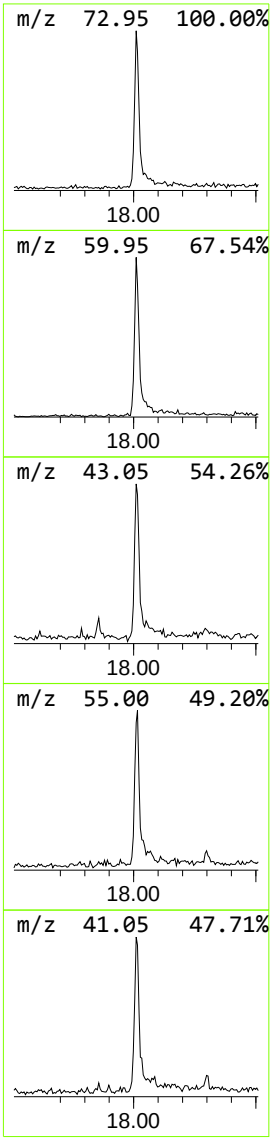
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.010	13.98 ng	188812	Phenanthrene-d10	17.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
3	Tridecanoic acid	214	C13H26O2	000638-53-9	60
4	Undecanoic acid	186	C11H22O2	000112-37-8	43
5	Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	22





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Operator : CG/JU
Sample : M1973-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BU-02-040721

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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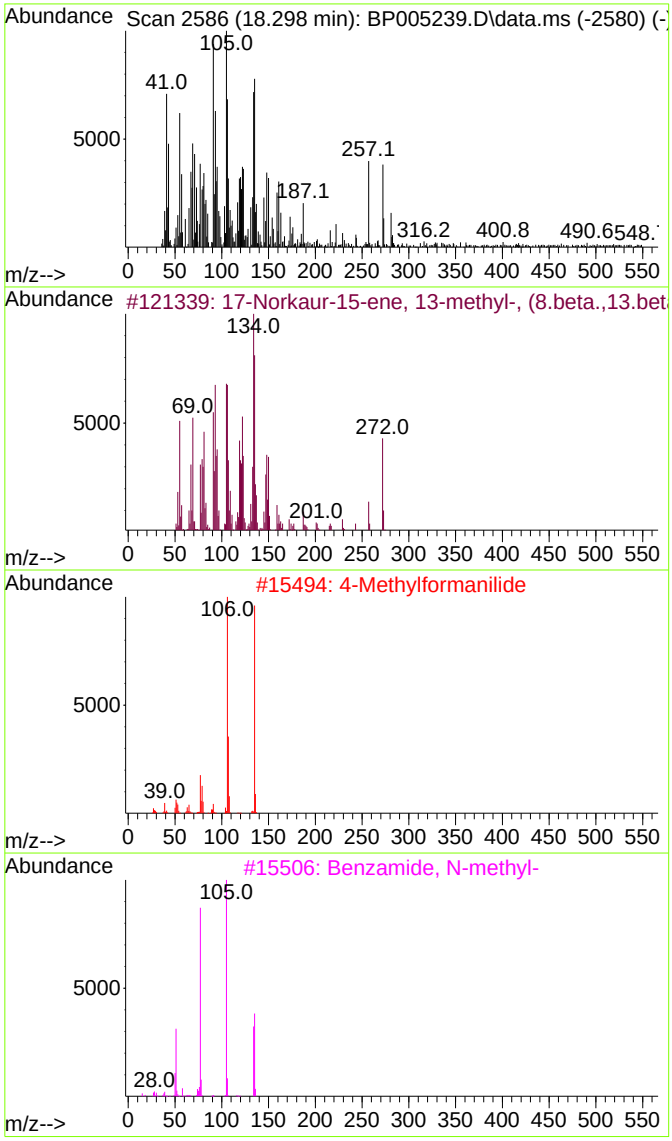
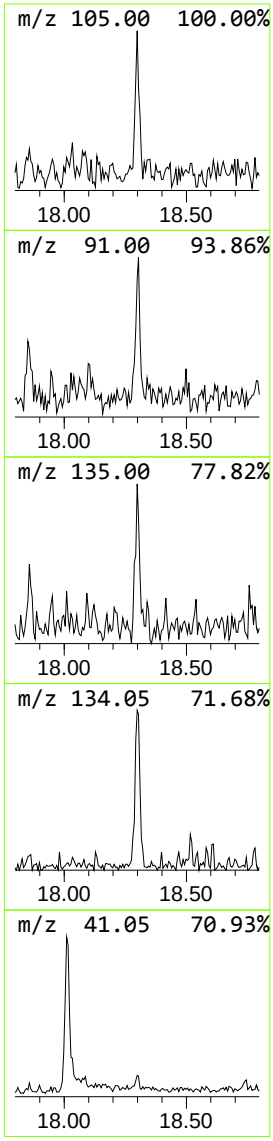
****
Peak Number 5 17-Norkaur-15-ene, 13-methy... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.298	2.01 ng	27158	Phenanthrene-d10	17.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Norkaur-15-ene, 13-methyl-, (...	272	C20H32	003564-54-3	95
2	4-Methylformanilide	135	C8H9NO	003085-54-9	46
3	Benzamide, N-methyl-	135	C8H9NO	000613-93-4	38
4	Benzenamine, N,N,4-trimethyl-	135	C9H13N	000099-97-8	35
5	Formamide, N-methyl-N-phenyl-	135	C8H9NO	000093-61-8	35





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Instrument :
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BU-02-040721

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

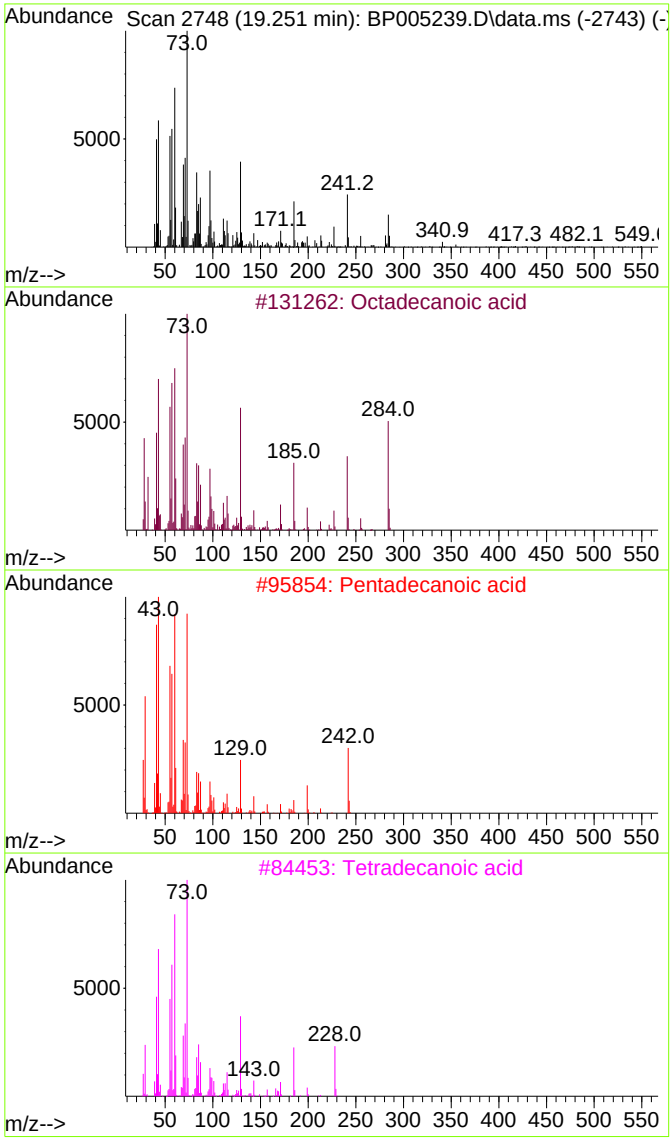
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

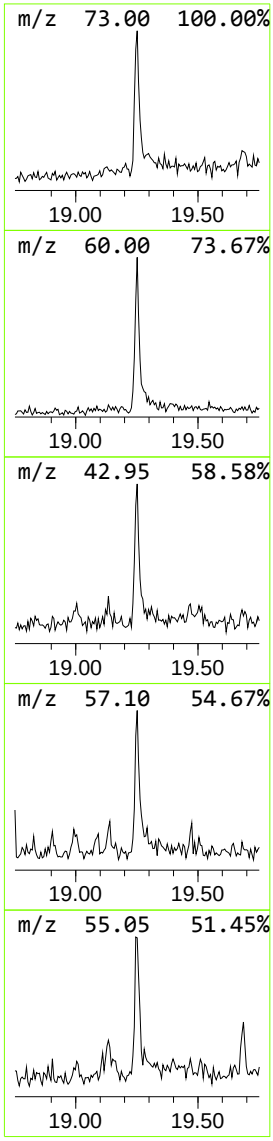
****

Peak Number 6 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.251	3.54 ng	83586	Chrysene-d12	21.210

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Tridecanoic acid	214	C13H26O2	000638-53-9	62





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

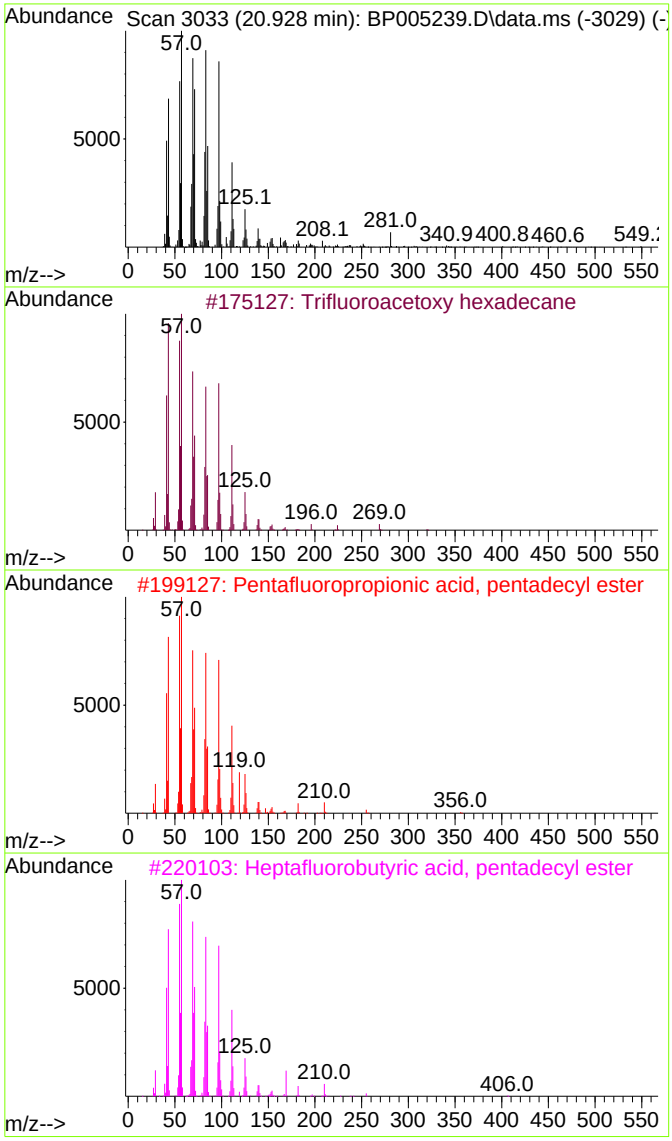
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

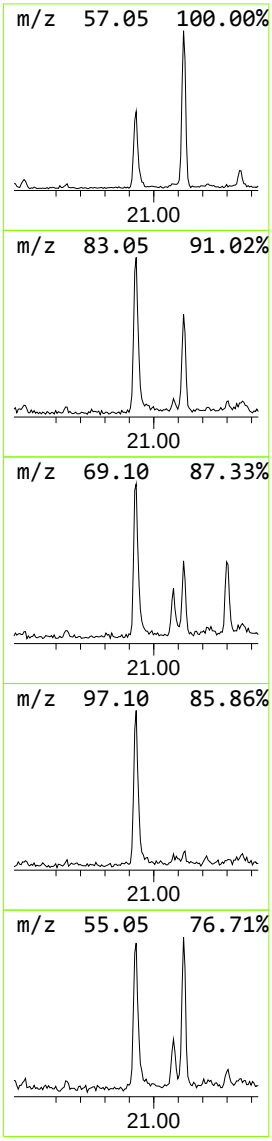
****

Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.927	9.70 ng	228898	Chrysene-d12	21.210

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
4	1-Heptacosanol	396	C27H56O	002004-39-9	90
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	87





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Data File : BP005239.D
Acq On : 08 Apr 2021 16:59
Operator : CG/JU
Sample : M1973-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BU-02-040721

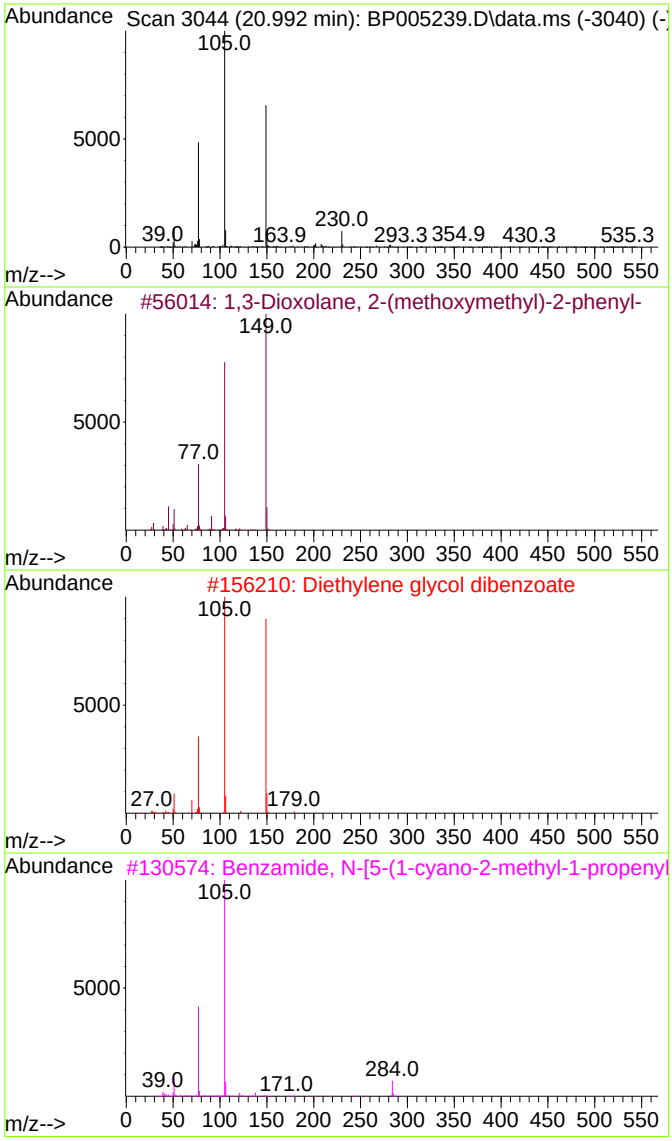
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

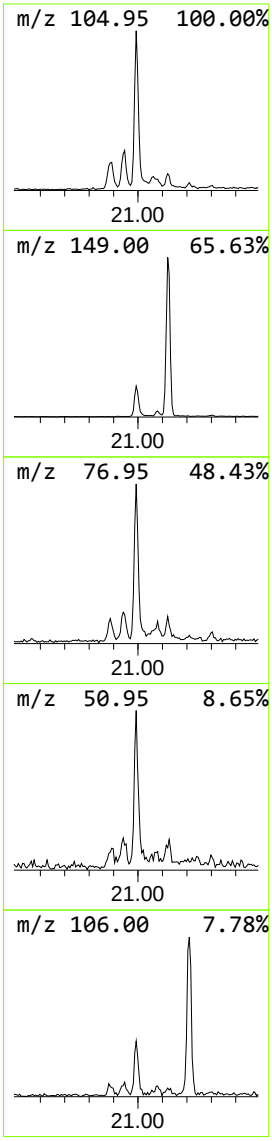
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.992	4.83 ng	113812	Chrysene-d12	21.210

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	72
2	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	53
3	Benzamide, N-[5-(1-cyano-2-methy...	284	C14H12N4OS	172535-11-4	43
4	2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	43
5	4'-Chlorobenzanilide	231	C13H10ClNO	002866-82-2	38





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Data File : BP005239.D
Acq On : 08 Apr 2021 16:59
Operator : CG/JU
Sample : M1973-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BU-02-040721

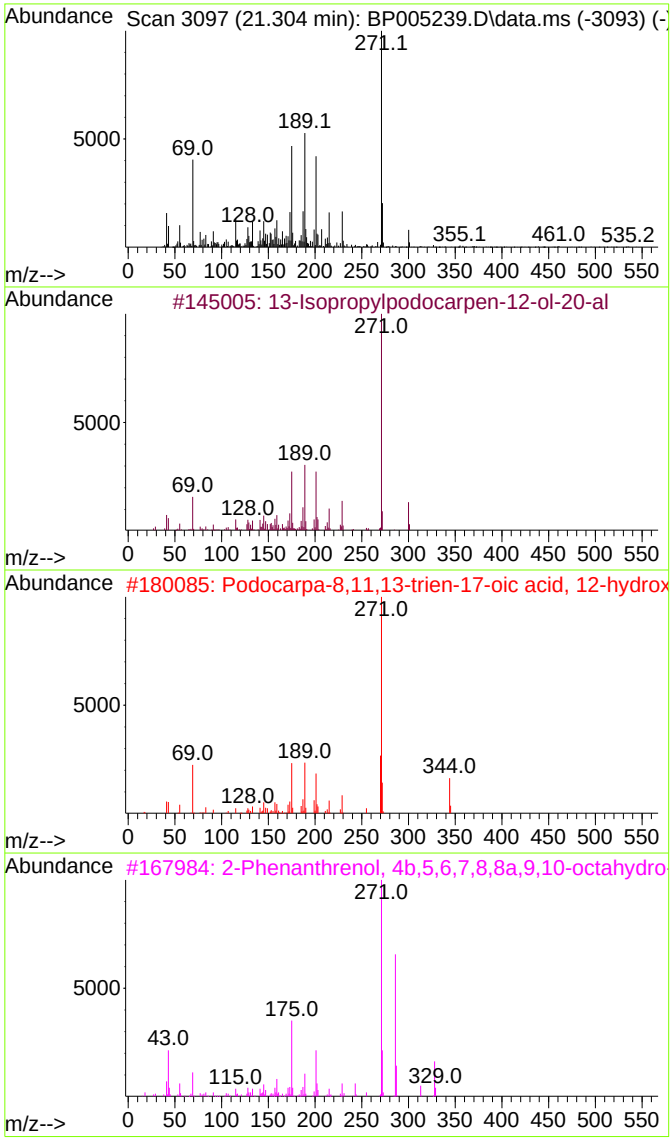
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

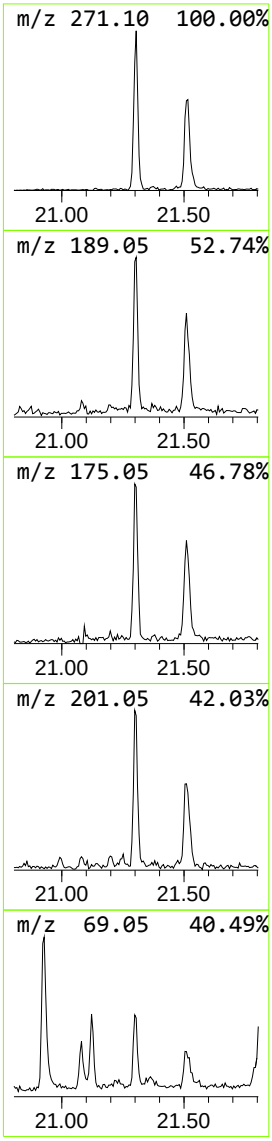
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 13-Isopropylpodocarpen-12-o... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.304	5.34 ng	125938	Chrysene-d12	21.210

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Isopropylpodocarpen-12-ol-20-al	300	C20H28O2	024035-37-8	90
2	Podocarpa-8,11,13-trien-17-oic a...	344	C22H32O3	024067-43-4	47
3	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	328	C22H32O2	015340-82-6	42
4	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	38
5	(-)-Morphinan-6-one, 4-methoxy-	271	C17H21NO2	1000129-09-1	30





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Operator : CG/JU
Sample : M1973-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BU-02-040721

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

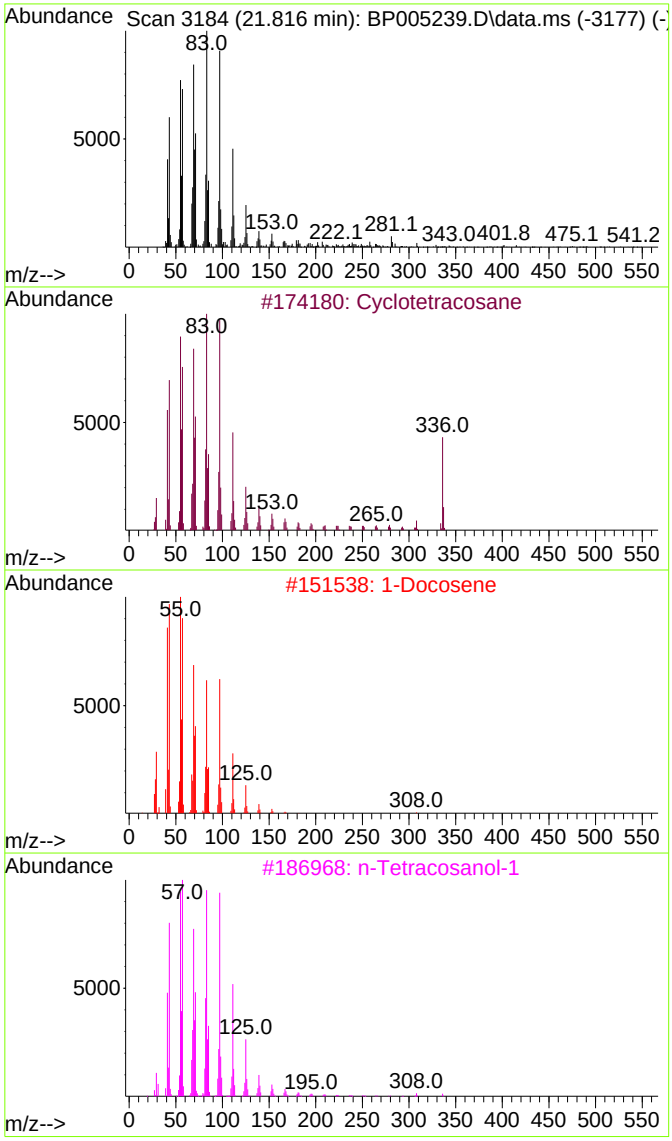
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

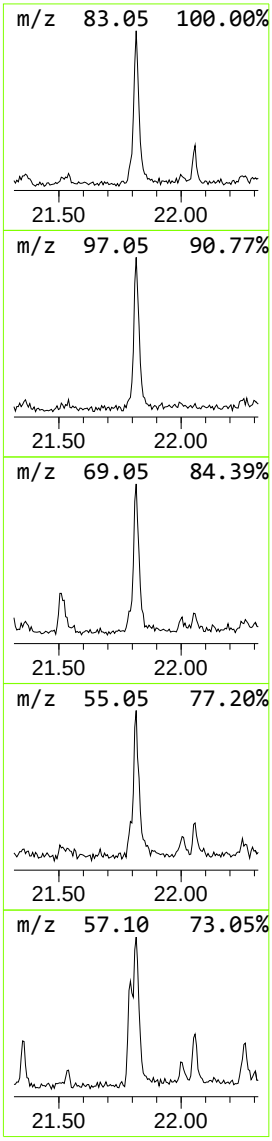
****

Peak Number 11 Cyclotetracosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.816	11.61 ng	273806	Chrysene-d12	21.210

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	95
2	1-Docosene	308	C22H44	001599-67-3	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	1-Heptacosanol	396	C27H56O	002004-39-9	93





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Data File : BP005239.D
Acq On : 08 Apr 2021 16:59
Operator : CG/JU
Sample : M1973-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BU-02-040721

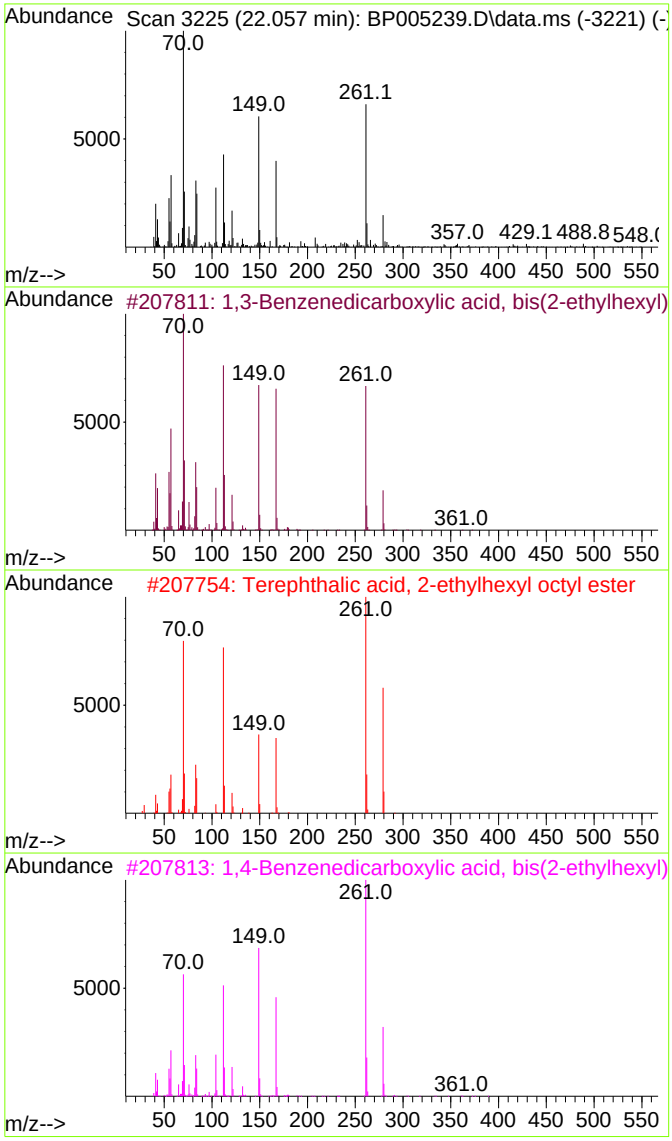
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

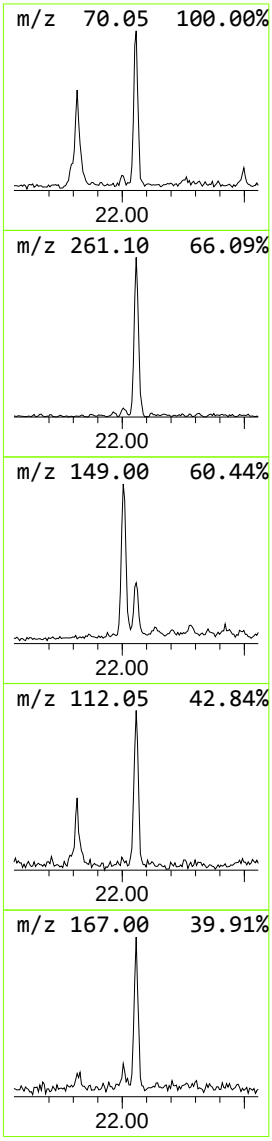
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 1,3-Benzenedicarboxylic aci... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.057	3.05 ng	71934	Chrysene-d12	21.210

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	50
2	Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	47
3	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	38
4	Terephthalic acid, 3-hexyl octyl...	362	C22H34O4	1000356-23-1	35
5	Cyclohexaneamine, N-but-2-enylid...	167	C10H17NO	068048-01-1	27





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Instrument :
BNA_P
ClientSampleId :
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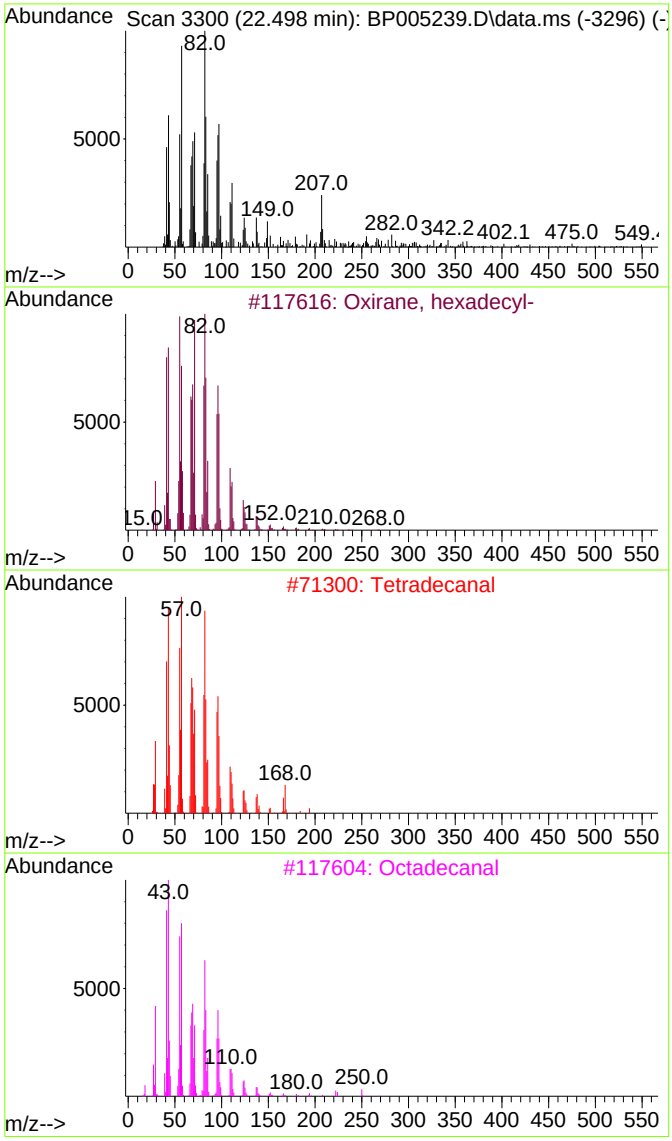
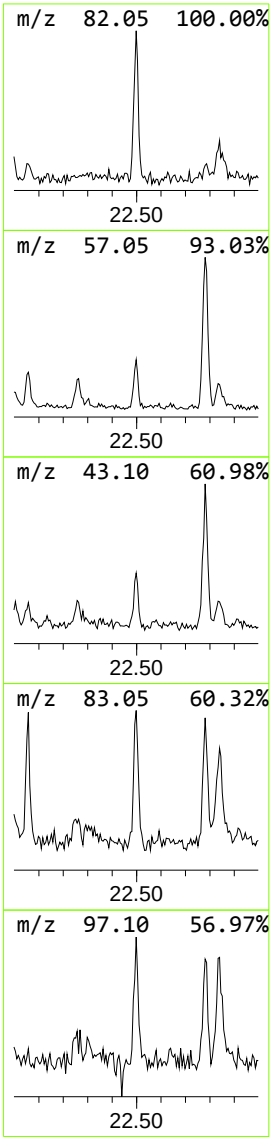
Peak Number 13 Oxirane, hexadecyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.498	3.29 ng	72717	Perylene-d12	23.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	86
2	Tetradecanal	212	C14H28O	000124-25-4	81
3	Octadecanal	268	C18H36O	000638-66-4	72
4	trans-2-Dodecen-1-ol	184	C12H24O	069064-37-5	62
5	1,19-Eicosadiene	278	C20H38	014811-95-1	60





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Operator : CG/JU
Sample : M1973-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BU-02-040721

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.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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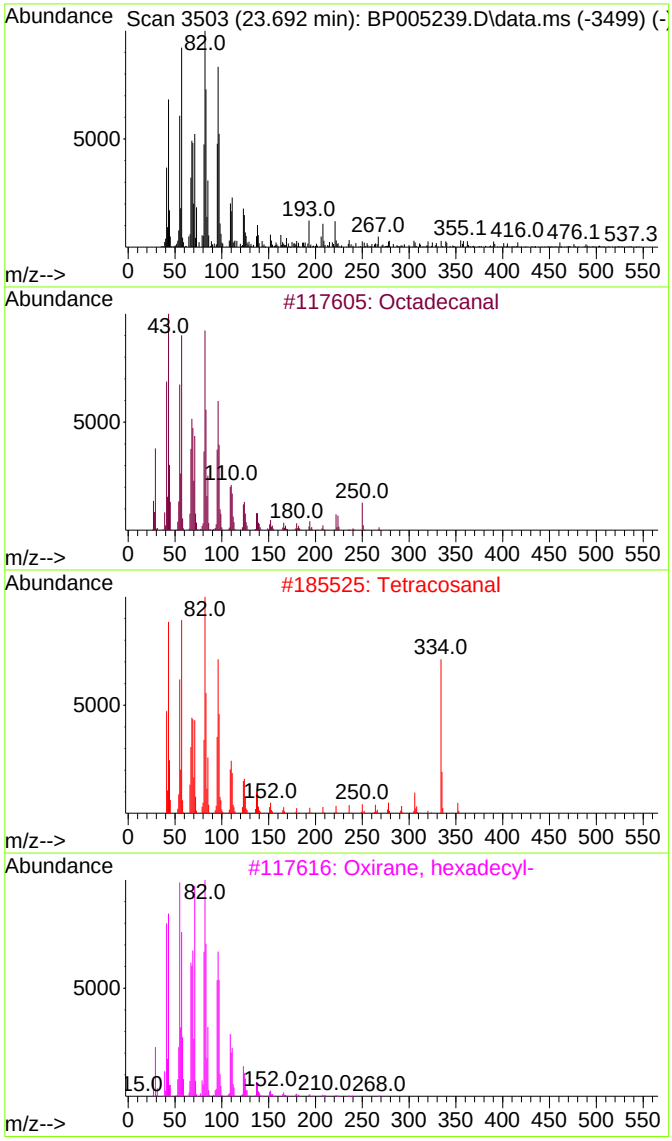
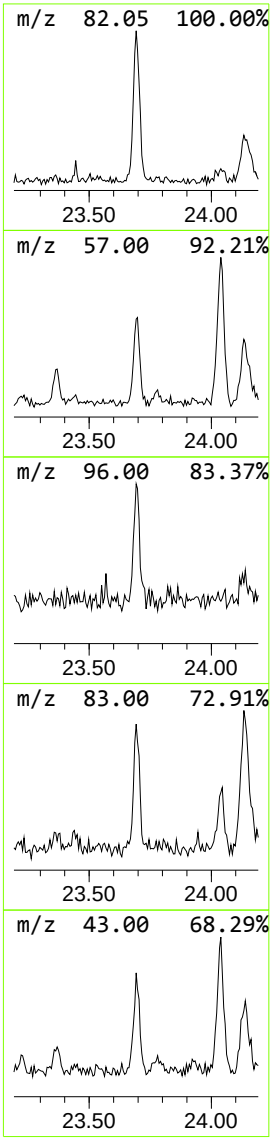
Peak Number 14 Octadecanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.692	5.35 ng	118357	Perylene-d12	23.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	91
2	Tetracosanal	352	C24H48O	057866-08-7	90
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	80
4	16-Heptadecenal	252	C17H32O	1000144-57-9	72
5	Hexadecanal	240	C16H32O	000629-80-1	64





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Sample : M1973-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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

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TIC Integration Parameters: LSCINT.P

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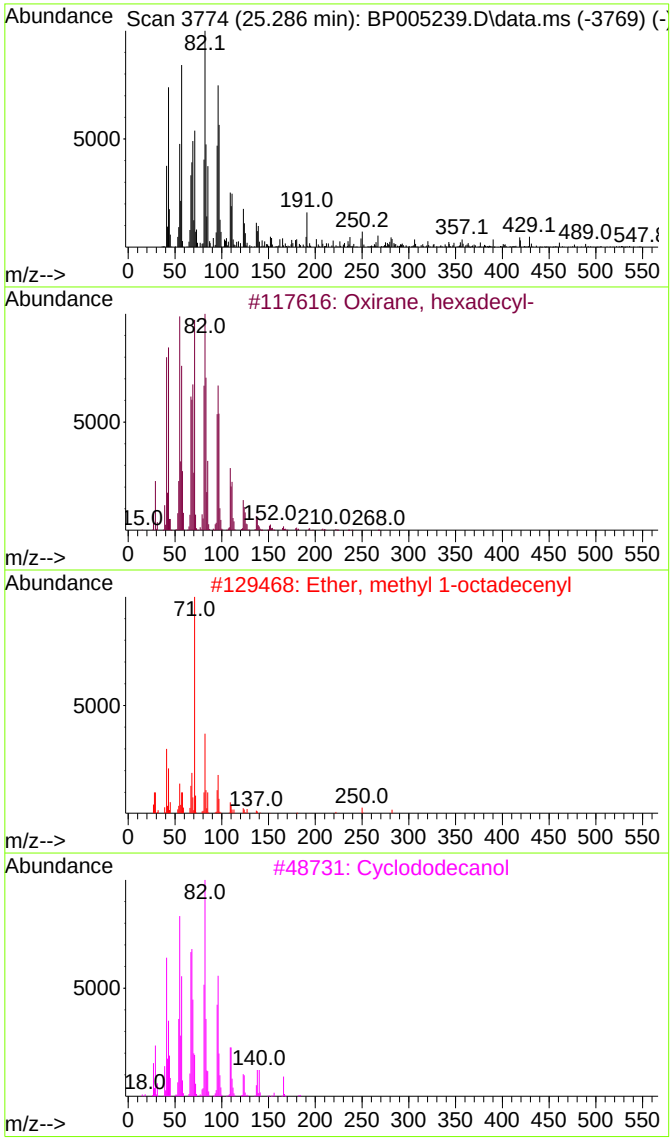
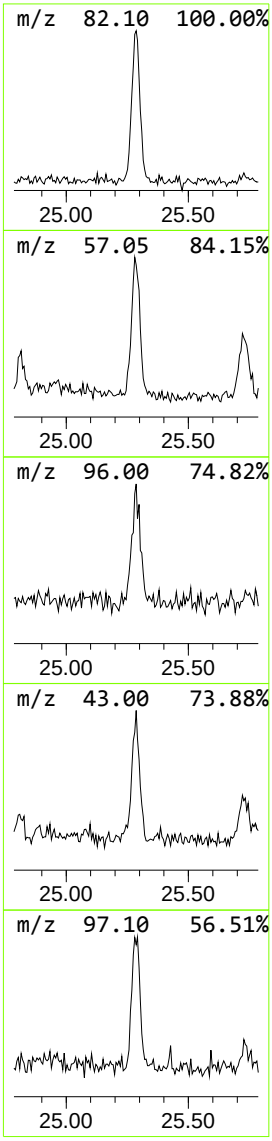
Peak Number 15 Ether, methyl 1-octadecenyl Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.286	7.19 ng	159012	Perylene-d12	23.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	80
2	Ether, methyl 1-octadecenyl	282	C19H38O	026537-06-4	74
3	Cyclododecanol	184	C12H24O	001724-39-6	70
4	17-Octadecenal	266	C18H34O	056554-86-0	68
5	Z-14-Octadecen-1-ol acetate	310	C20H38O2	1000131-07-6	64





Tentatively Identified Compound (LSC) summary

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Data File : BP005239.D
Acq On : 08 Apr 2021 16:59
Operator : CG/JU
Sample : M1973-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BU-02-040721

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(1R)-2,6,6-Trim...	6.369	11.0	ng	72767	1	7.687	132698	20.0
3-Carene	7.581	4.3	ng	28403	1	7.687	132698	20.0
Bornyl acetate	11.846	5.3	ng	44959	2	10.475	168292	20.0
n-Hexadecanoic ...	18.010	14.0	ng	188812	4	17.110	270091	20.0
17-Norkaur-15-e...	18.298	2.0	ng	27158	4	17.110	270091	20.0
Octadecanoic acid	19.251	3.5	ng	83586	5	21.210	471734	20.0
Trifluoroacetox...	20.927	9.7	ng	228898	5	21.210	471734	20.0
1,3-Dioxolane, ...	20.992	4.8	ng	113812	5	21.210	471734	20.0
13-Isopropylpod...	21.304	5.3	ng	125938	5	21.210	471734	20.0
Cyclotetracosane	21.816	11.6	ng	273806	5	21.210	471734	20.0
1,3-Benzenedica...	22.057	3.0	ng	71934	5	21.210	471734	20.0
Oxirane, hexade...	22.498	3.3	ng	72717	6	23.486	442548	20.0
Octadecanal	23.692	5.3	ng	118357	6	23.486	442548	20.0
Ether, methyl 1...	25.286	7.2	ng	159012	6	23.486	442548	20.0