LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008247.D
Acq On : 07 Dec 2021 12:35
Operator : CG/JU
Sample : M4927-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PH1-BOT-5

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-BP112521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008247.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.910	322	327	334	rBV	46946	70537	2.01%	0.414%
2	5.381	400	407	425	rBV	902021	1397543	39.87%	8.198%
3	6.975	668	678	689	rBV	876066	1484220	42.35%	8.706%
4	7.787	807	816	823	rBV	186442	301078	8.59%	1.766%
5	8.945	1006	1013	1023	rBV	542096	915255	26.11%	5.369%
6	10.386	1251	1258	1268	rBV2	25586	54442	1.55%	0.319%
7	10.581	1284	1291	1302	rBV	231215	406084	11.59%	2.382%
8	13.057	1705	1712	1725	rBV	1280460	1965183	56.07%	11.527%
9	14.098	1882	1889	1896	rBV2	20488	35771	1.02%	0.210%
10	14.433	1940	1946	1960	rBV	348481	541985	15.46%	3.179%
11	15.939	2195	2202	2211	rBV	1055266	1585621	45.24%	9.301%
12	17.127	2399	2404	2409	rBV5	27682	36918	1.05%	0.217%
13	17.198	2410	2416	2426	rVV	464887	680168	19.41%	3.990%
14	18.098	2565	2569	2577	rBV	228903	341048	9.73%	2.001%
15	19.339	2776	2780	2788	rBV	181682	267442	7.63%	1.569%
16	19.774	2848	2854	2860	rBV	2772364	3505024	100.00%	20.560%
17	21.021	3062	3066	3071	rBV2	226496	365790	10.44%	2.146%
18	21.080	3072	3076	3080	rBV	386669	480711	13.71%	2.820%
19	21.304	3110	3114	3120	rBV	722010	982129	28.02%	5.761%
20	21.915	3215	3218	3226	rVB	107784	143437	4.09%	0.841%
21	22.415	3300	3303	3308	rVB	150334	194022	5.54%	1.138%
22	22.551	3324	3326	3333	rVB2	139563	179711	5.13%	1.054%
23	23.703	3516	3522	3530	rVB2	541452	1113744	31.78%	6.533%

Sum of corrected areas: 17047863

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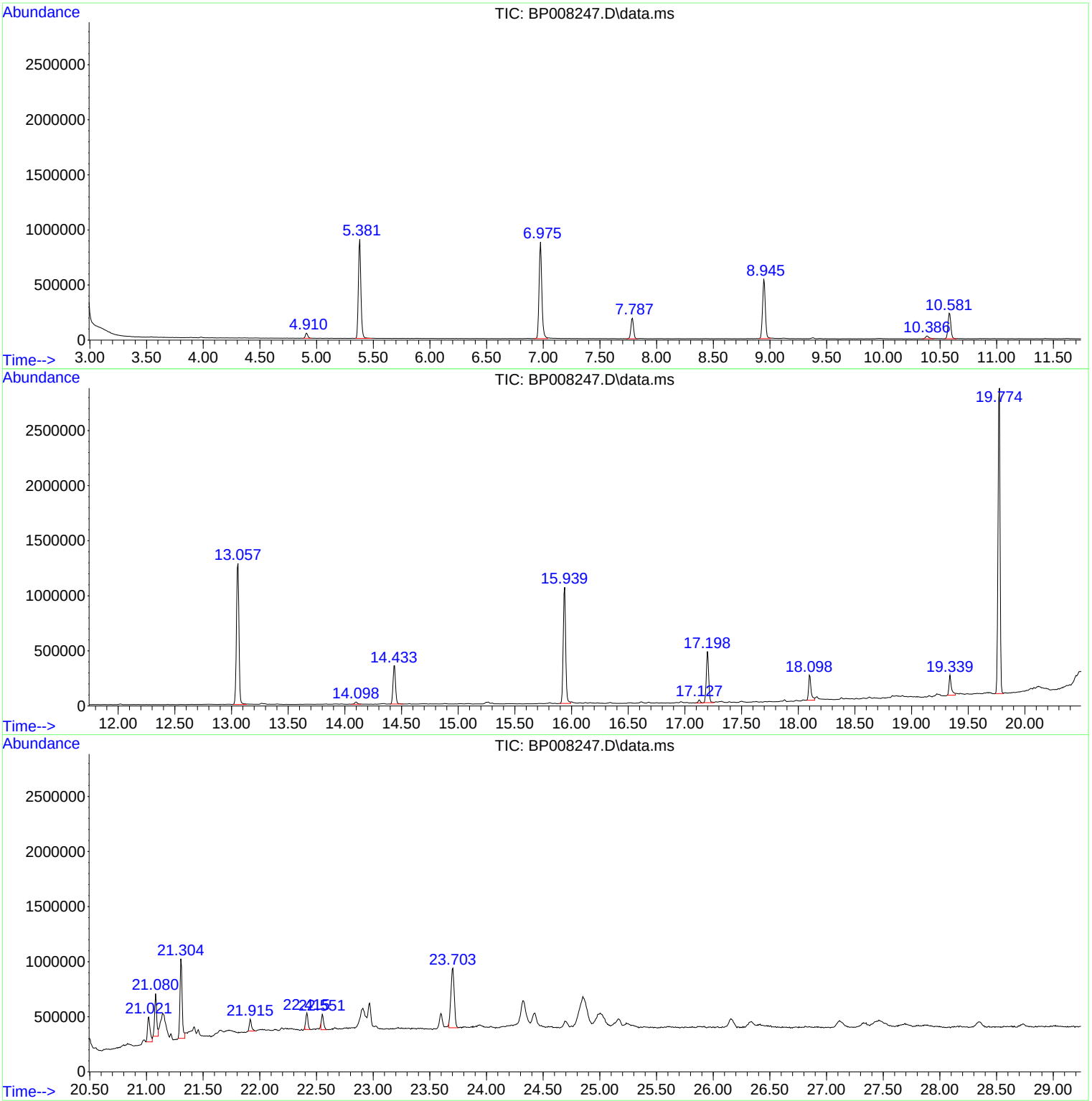
Instrument :
BNA_P
ClientSampleId :
PH1-BOT-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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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Data File : BP008247.D
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ClientSampleId :
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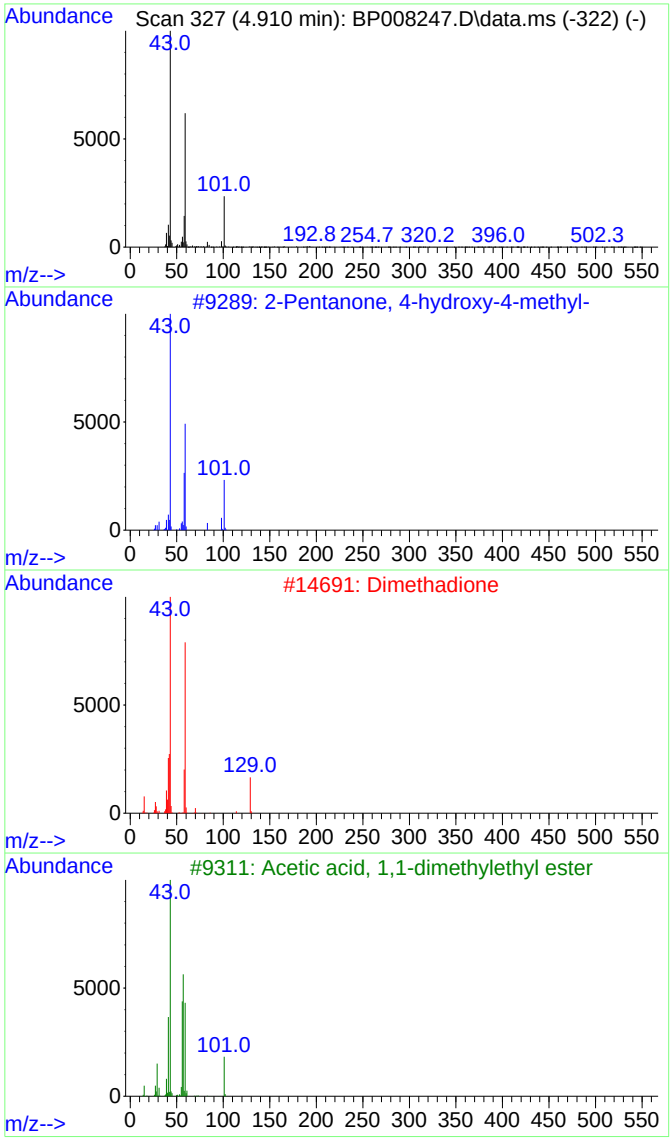
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

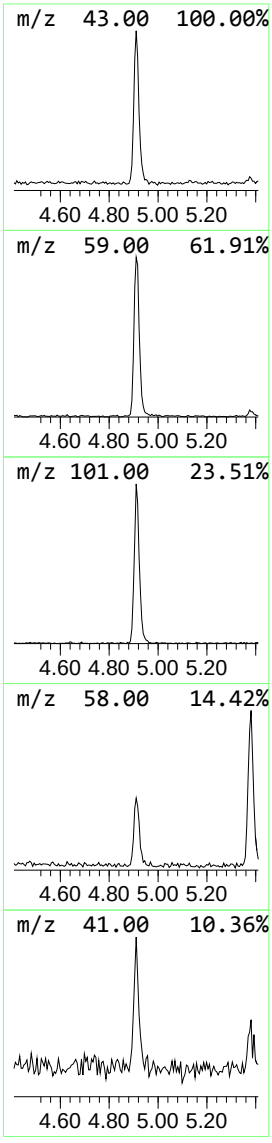
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.910	4.69 ng	70537	1,4-Dichlorobenzene-d4	7.787

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Dimethadione	129	C5H7NO3	000695-53-4	40
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4	Tripropylene glycol, propyl ethe...	348	C18H40O4Si	1000367-07-2	28
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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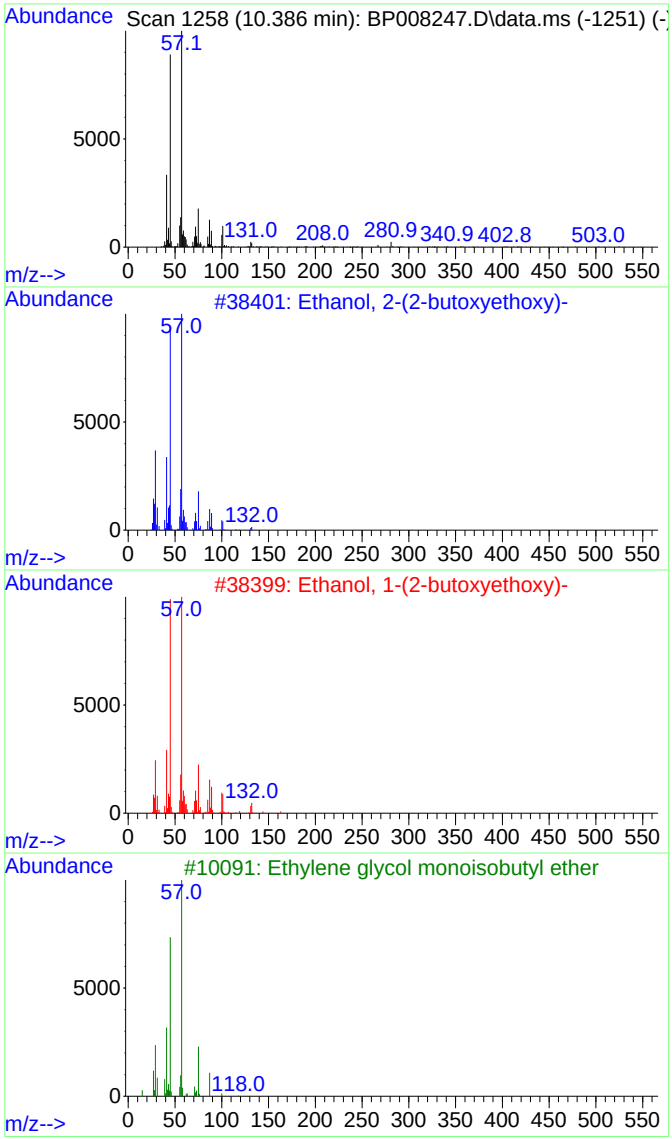
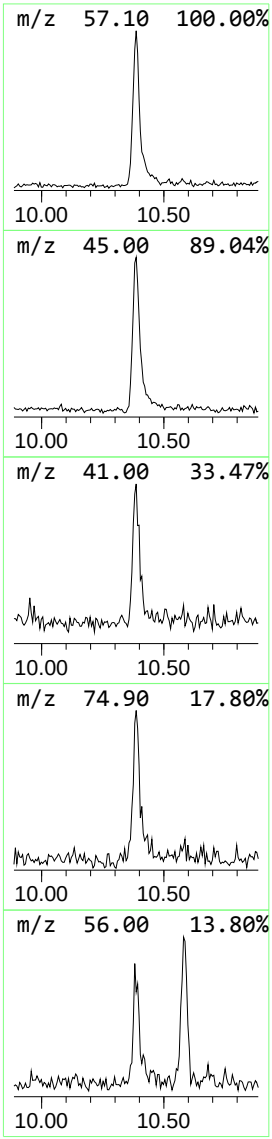
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.387	2.68 ng	54442	Naphthalene-d8	10.581

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	80
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	72
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	68
4	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	59
5	Butane, 1,1'-[ethylidenebis(oxy)...	174	C10H22O2	000871-22-7	53





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Sample : M4927-03
Misc :
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Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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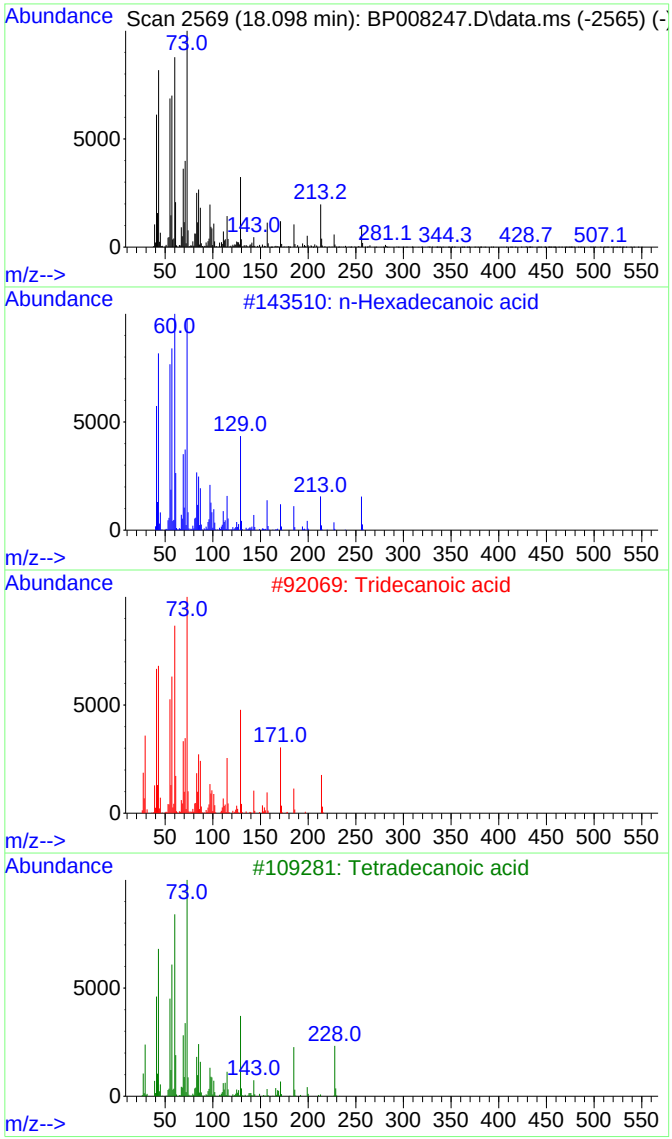
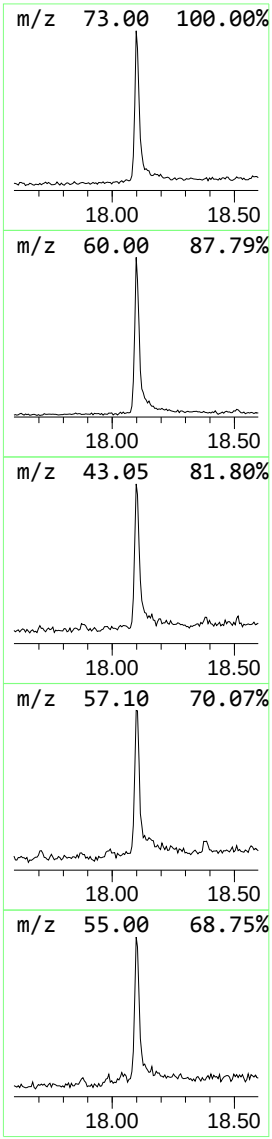
Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.098	10.03 ng	341048	Phenanthrene-d10	17.198

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	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	76





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Instrument :
BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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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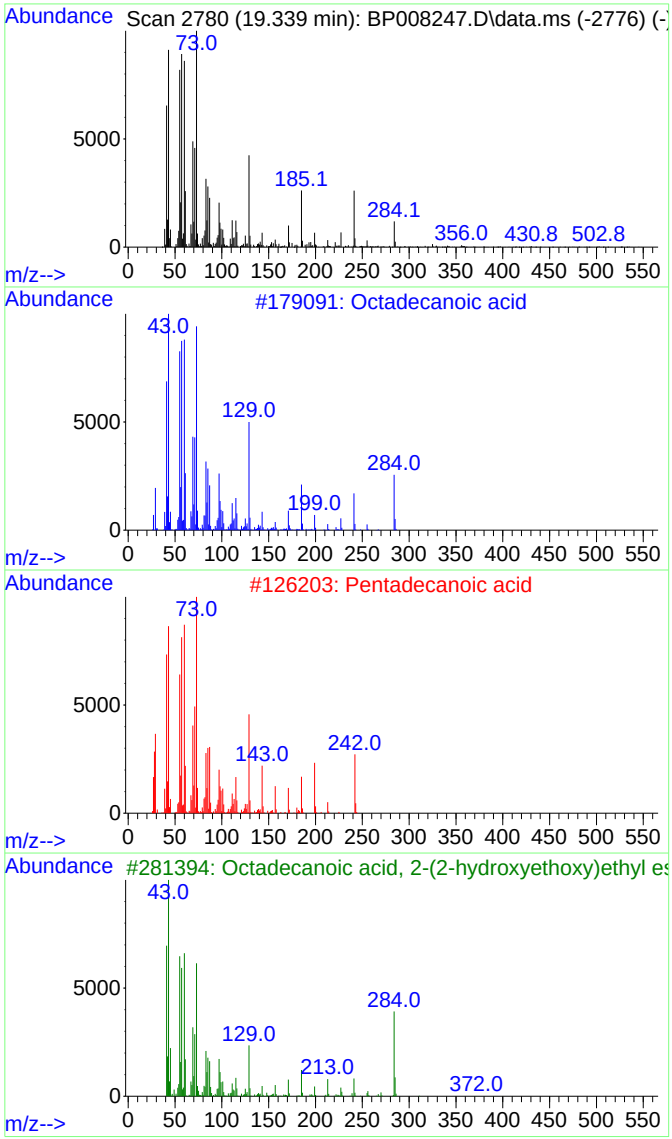
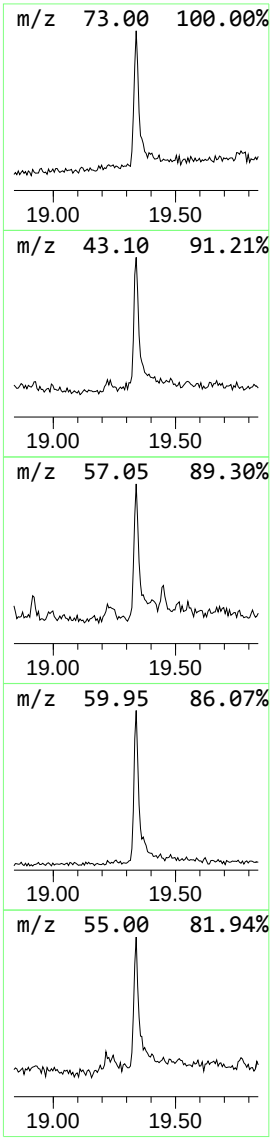
Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.339	5.45 ng	267442	Chrysene-d12	21.304

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	91
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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Data File : BP008247.D
Acq On : 07 Dec 2021 12:35
Operator : CG/JU
Sample : M4927-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PH1-BOT-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

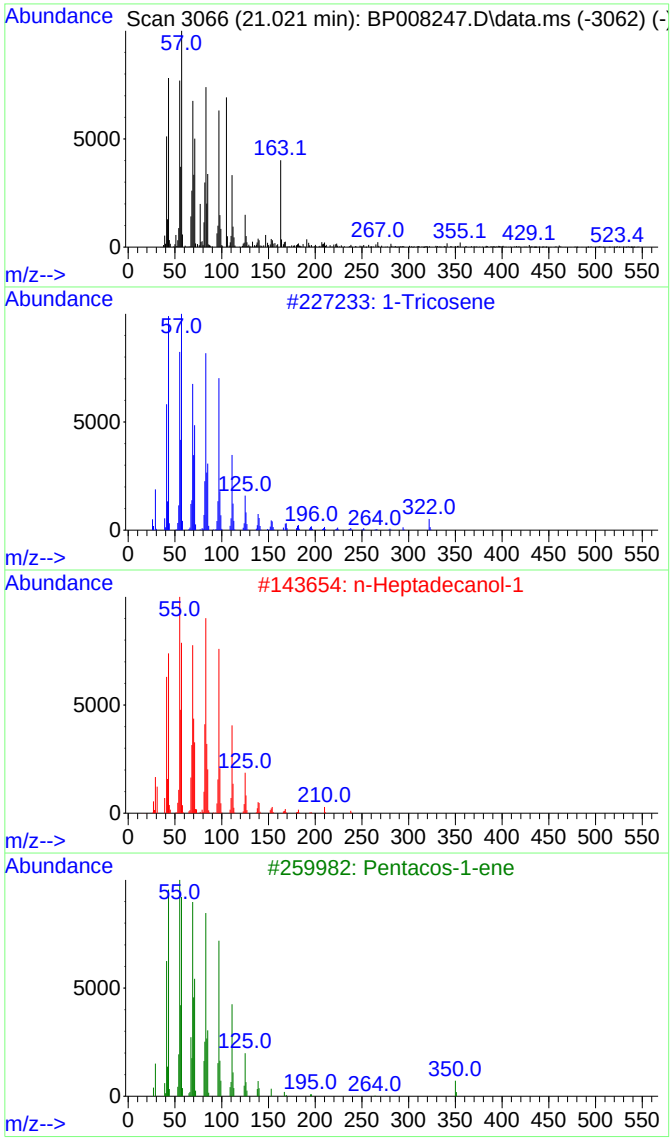
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

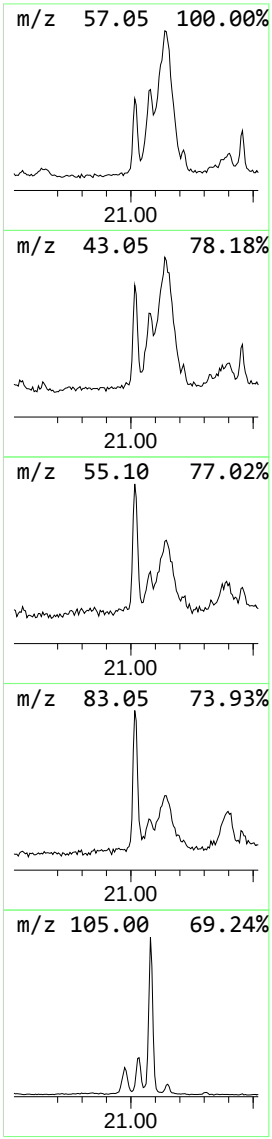
****

Peak Number 5 1-Tricosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.021	7.45 ng	365790	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	93
2	n-Heptadecanol-1	256	C17H36O	001454-85-9	92
3	Pentacos-1-ene	350	C25H50	016980-85-1	90
4	1-Triacontanol	438	C30H62O	000593-50-0	90
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	89





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Operator : CG/JU
Sample : M4927-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PH1-BOT-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

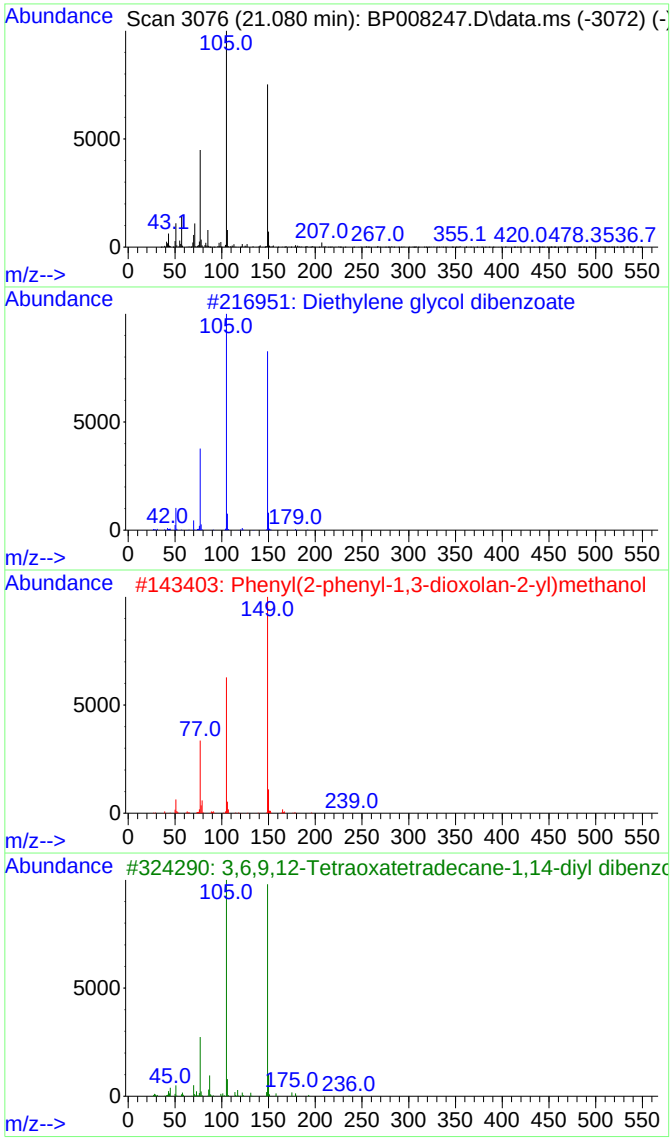
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

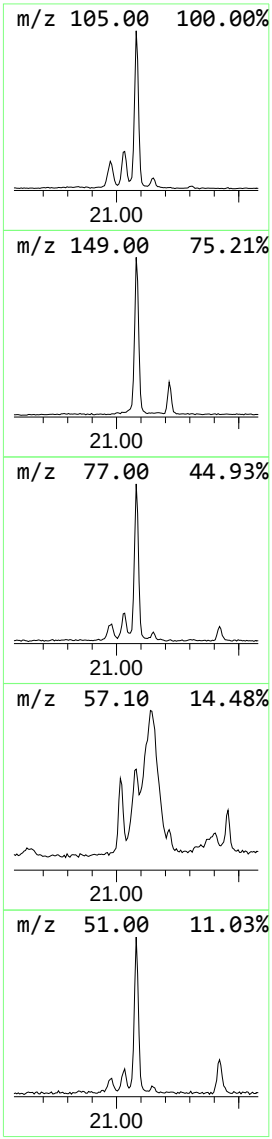
****

Peak Number 6 Diethylene glycol dibenzoate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.080	9.79 ng	480711	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	80
2	Phenyl(2-phenyl-1,3-dioxolan-2-y...	256	C16H16O3	005694-69-9	64
3	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	59
4	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	59
5	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	59





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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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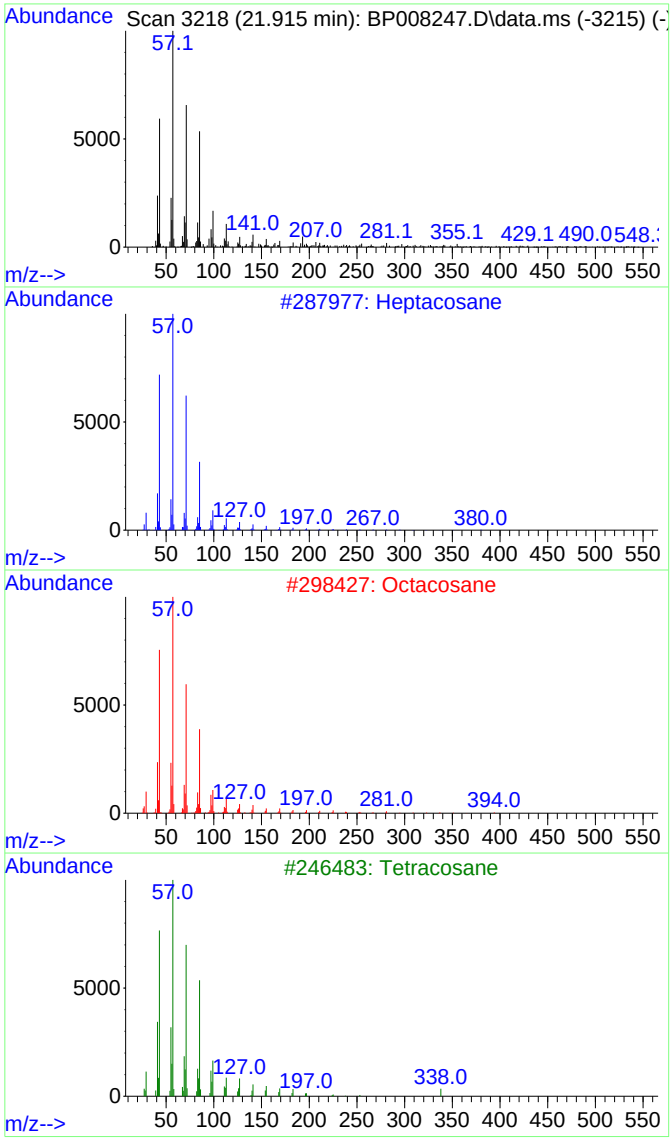
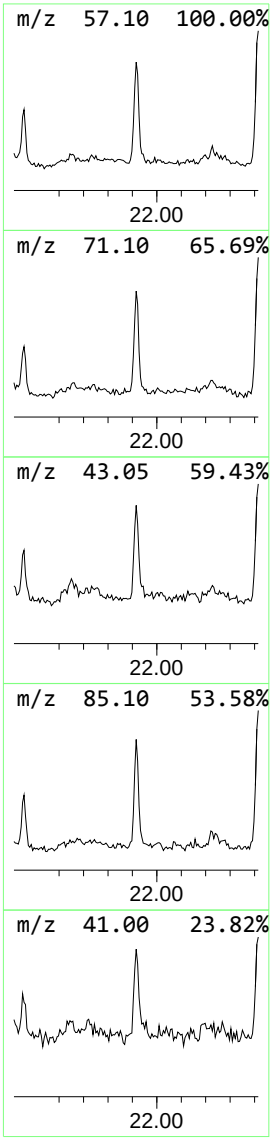
Peak Number 7 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.915	2.92 ng	143437	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	98
2	Octacosane	394	C28H58	000630-02-4	90
3	Tetracosane	338	C24H50	000646-31-1	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	87





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BNA_P
ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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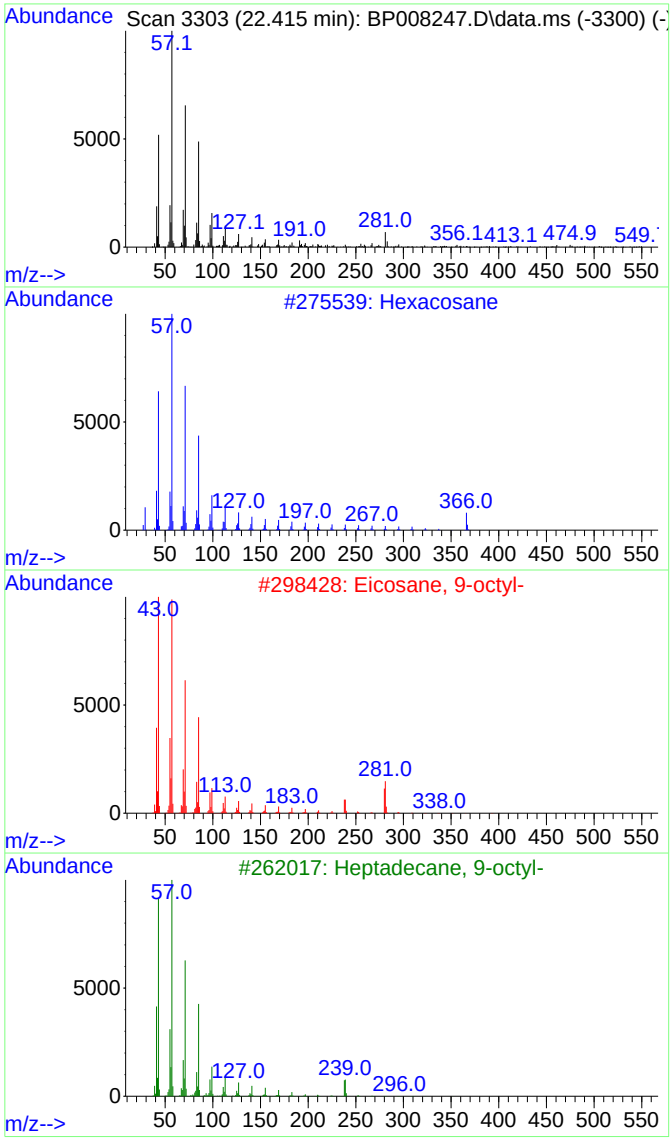
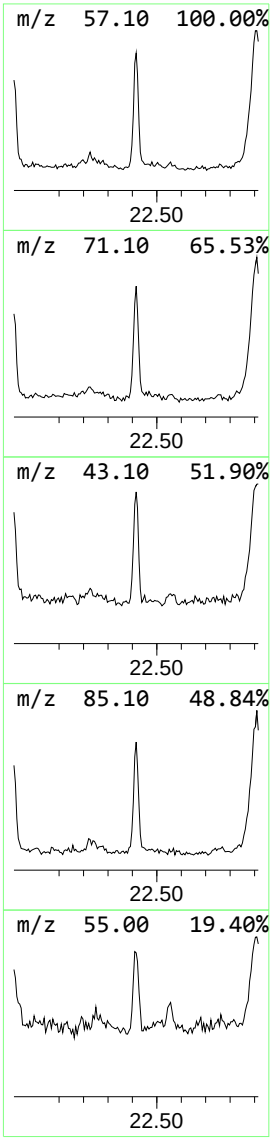
Peak Number 8 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.415	3.95 ng	194022	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	97
2	Eicosane, 9-octyl-	394	C28H58	013475-77-9	90
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	81
4	Heneicosane	296	C21H44	000629-94-7	81
5	Tetracosane	338	C24H50	000646-31-1	81





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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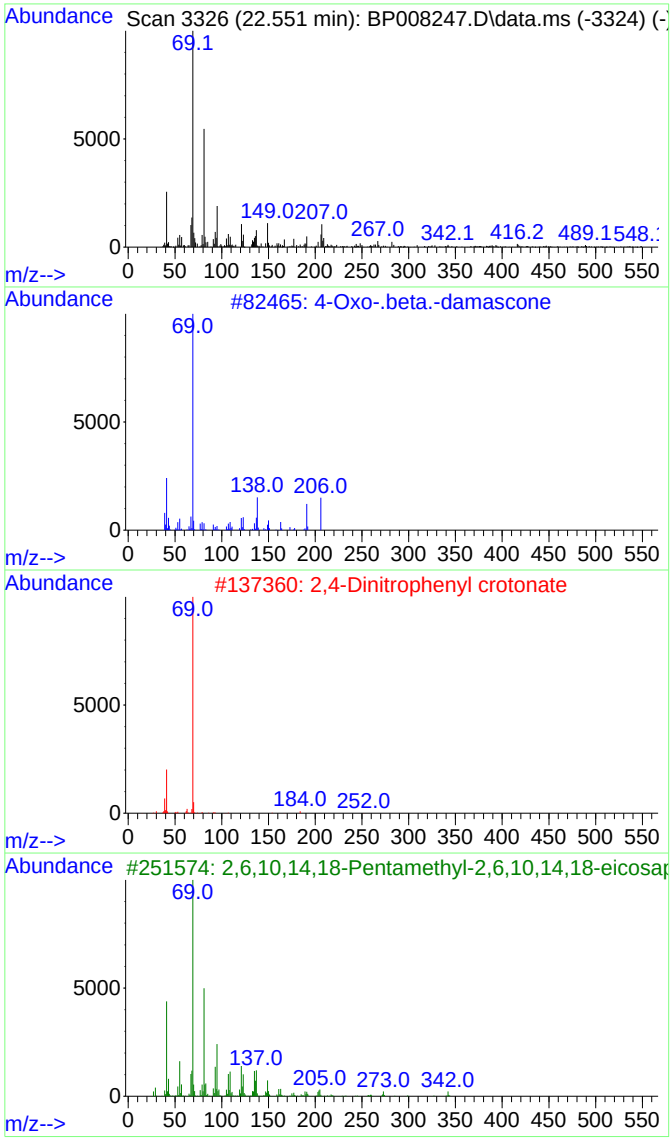
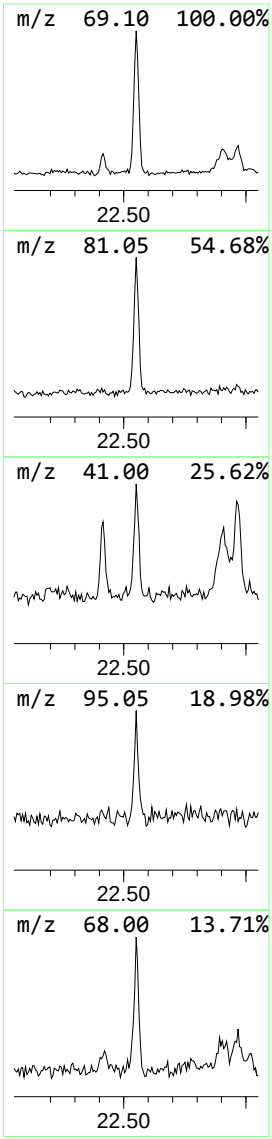
Peak Number 9 4-Oxo-.beta.-damascone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.551	3.23 ng	179711	Perylene-d12	23.703

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Oxo-.beta.-damascone	206	C13H18O2	053398-08-6	53
2	2,4-Dinitrophenyl crotonate	252	C10H8N2O6	069817-88-5	53
3	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	53
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	53
5	1-(Pyrrolidin-3-yl)pyrazole	137	C7H11N3	1000459-08-8	53





Tentatively Identified Compound (LSC) summary

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Operator : CG/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	4.910	4.7	ng	70537	1	7.787	301078	20.0
Ethanol, 2-(2-b...	10.387	2.7	ng	54442	2	10.581	406084	20.0
n-Hexadecanoic ...	18.098	10.0	ng	341048	4	17.198	680168	20.0
Octadecanoic acid	19.339	5.5	ng	267442	5	21.304	982129	20.0
1-Tricosene	21.021	7.5	ng	365790	5	21.304	982129	20.0
Diethylene glyc...	21.080	9.8	ng	480711	5	21.304	982129	20.0
Heptacosane	21.915	2.9	ng	143437	5	21.304	982129	20.0
Hexacosane	22.415	4.0	ng	194022	5	21.304	982129	20.0
4-Oxo-.beta.-da...	22.551	3.2	ng	179711	6	23.703	1113740	20.0