LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE111224\
Data File : BE101590.D
Acq On : 12 Nov 2024 23:58
Operator : RC/JU
Sample : P4795-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
LAW-23-00189

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_E\Methods\8270-BE110624.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BE101590.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.676	11	15	27	rVB	978321	1253136	42.72%	6.553%
2	2.781	28	33	43	rVB2	14642	36514	1.24%	0.191%
3	2.864	43	47	54	rBV	271462	353822	12.06%	1.850%
4	4.773	369	372	384	rBV	51708	83791	2.86%	0.438%
5	5.314	457	464	493	rBV	618853	1079641	36.80%	5.646%
6	6.941	734	741	762	rBV	572750	1145028	39.03%	5.988%
7	7.558	837	846	853	rBV	186425	304831	10.39%	1.594%
8	8.768	1044	1052	1068	rBV	424131	758031	25.84%	3.964%
9	10.320	1309	1316	1332	rBV	268873	480375	16.38%	2.512%
10	12.787	1728	1736	1744	rBV	1319033	1992061	67.91%	10.417%
11	13.898	1921	1925	1933	rVB2	21581	36542	1.25%	0.191%
12	14.168	1964	1971	1977	rVB	442522	669902	22.84%	3.503%
13	14.855	2085	2088	2096	rVB2	26798	47648	1.62%	0.249%
14	15.537	2200	2204	2208	rBV	112502	155066	5.29%	0.811%
15	15.678	2222	2228	2234	rBV	1089450	1627758	55.49%	8.512%
16	15.749	2236	2240	2246	rVB	70546	121061	4.13%	0.633%
17	16.906	2433	2437	2442	rVB	488660	646008	22.02%	3.378%
18	19.503	2874	2879	2885	rBV	2280167	2933499	100.00%	15.340%
19	21.072	3142	3146	3150	rVB	636081	748108	25.50%	3.912%
20	22.112	3319	3323	3331	rVB	425138	616582	21.02%	3.224%
21	22.323	3354	3359	3364	rVB	461014	662873	22.60%	3.466%
22	22.646	3410	3414	3428	rVB	221445	686996	23.42%	3.593%
23	23.357	3529	3535	3540	rBV	543583	1016759	34.66%	5.317%
24	23.422	3541	3546	3556	rVB	673954	1354209	46.16%	7.082%
25	23.992	3639	3643	3649	rVB3	177699	312654	10.66%	1.635%

Sum of corrected areas: 19122895

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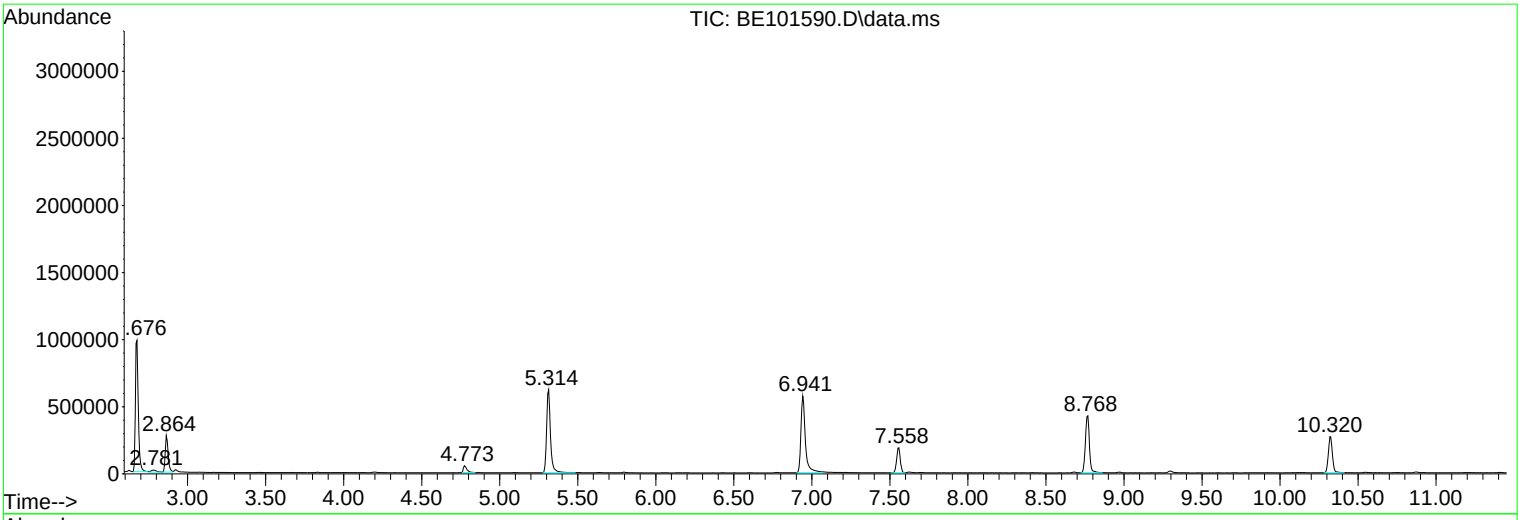
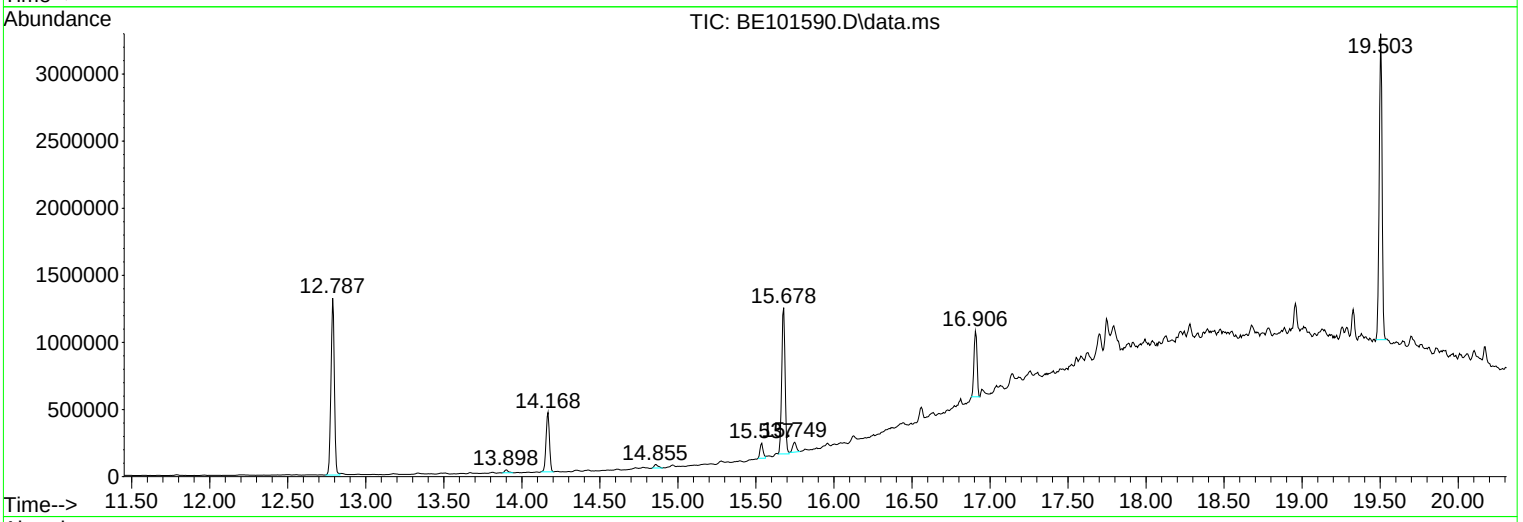
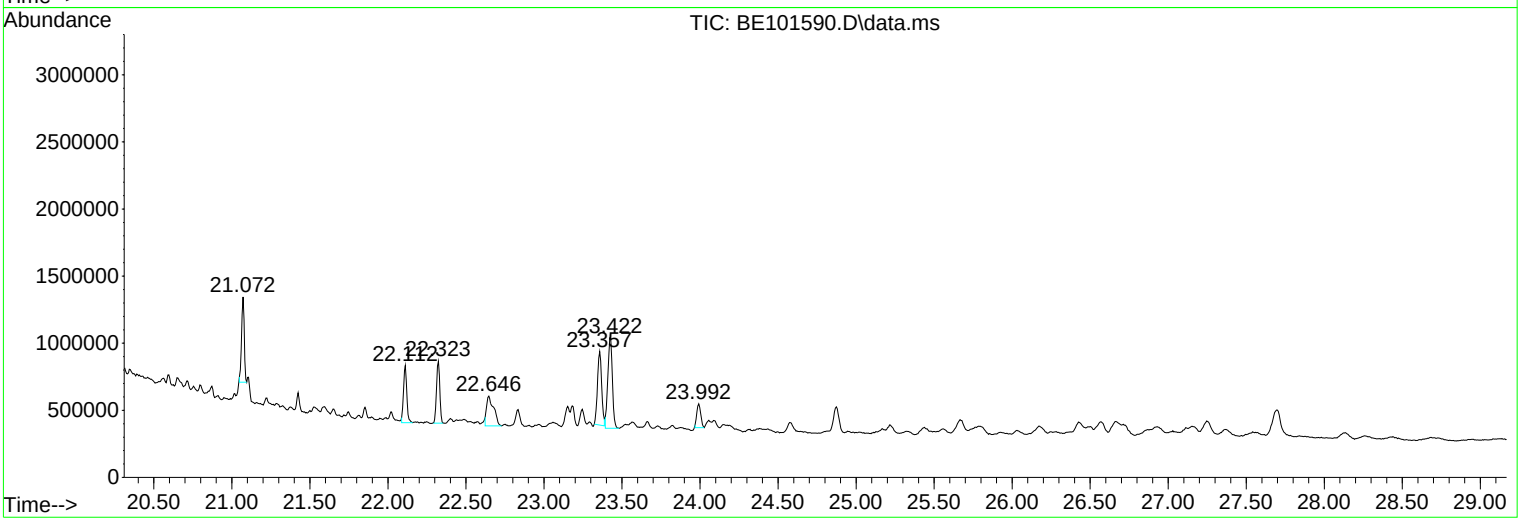
Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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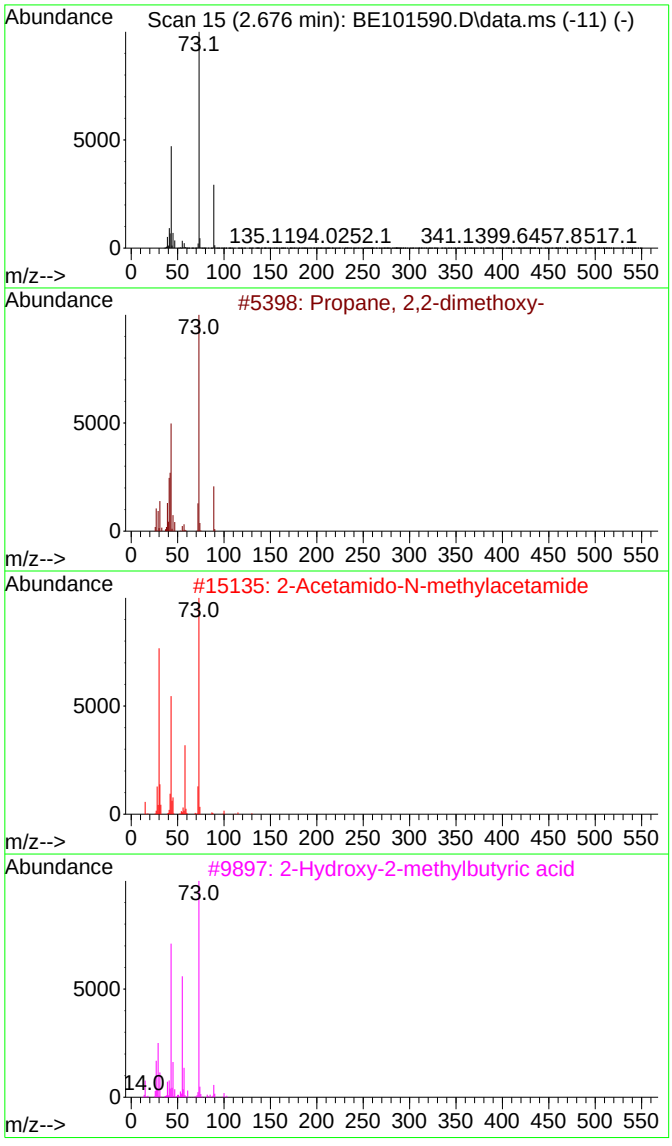
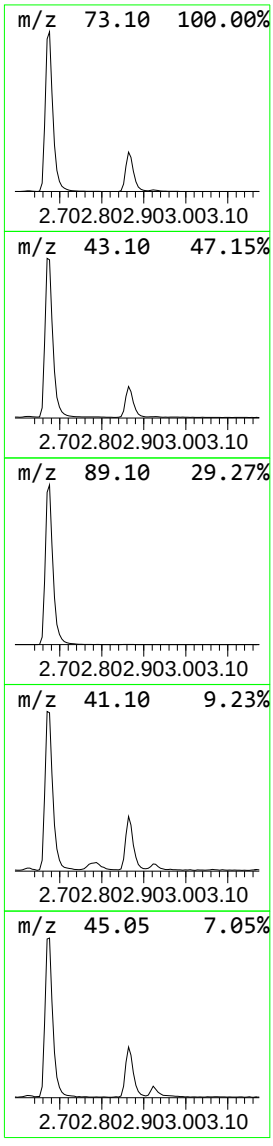
Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.676	82.22 ng	1253140	1,4-Dichlorobenzene-d4	7.558

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	9
3	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
4	1,3-Dioxolane, 2-hexyl-	158	C9H18O2	001708-34-5	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9





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

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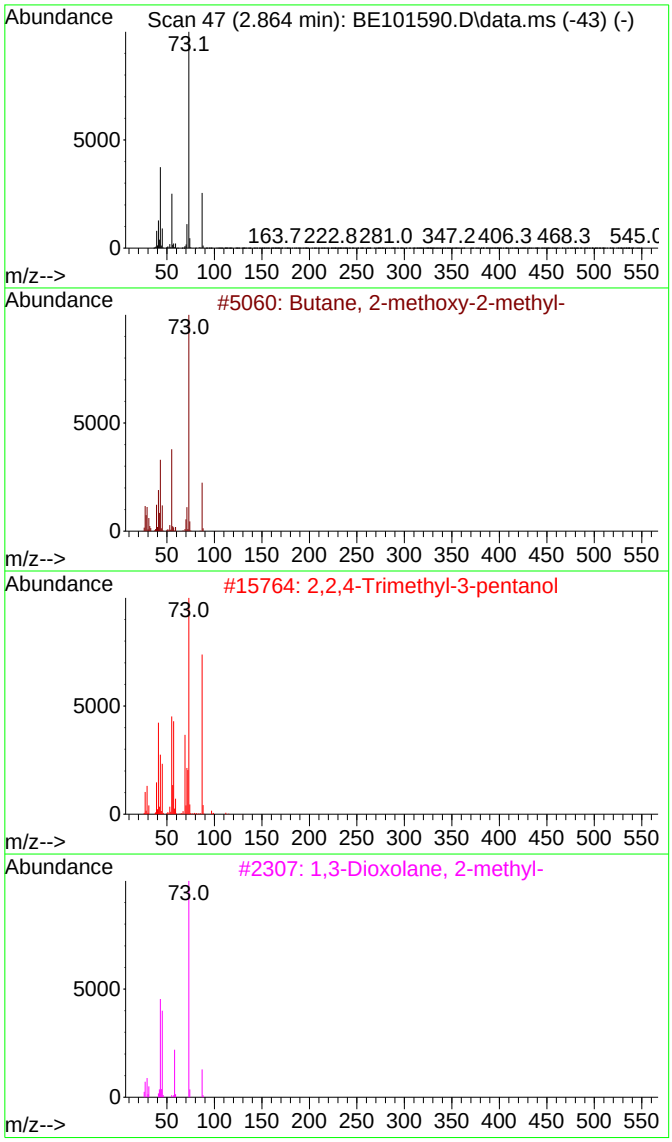
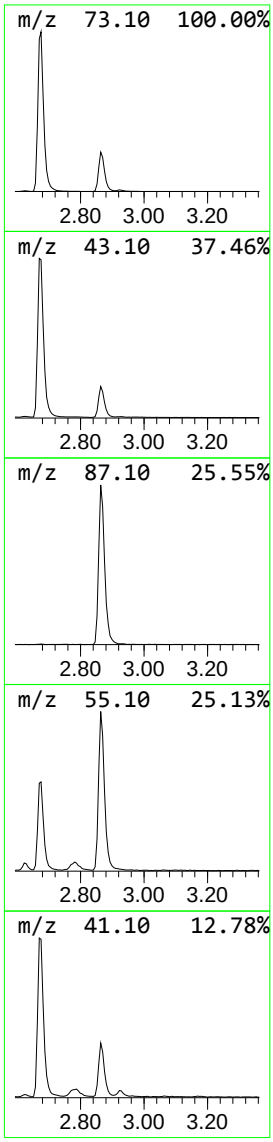
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.864	23.21 ng	353822	1,4-Dichlorobenzene-d4	7.558

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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BNA_E
ClientSampleId :
LAW-23-00189

Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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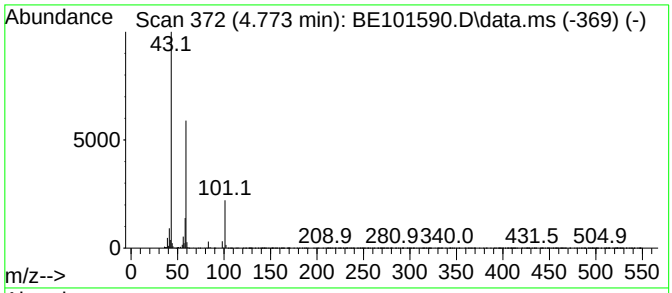
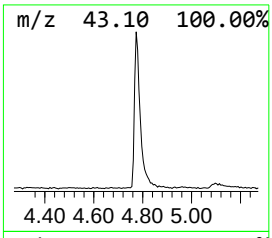
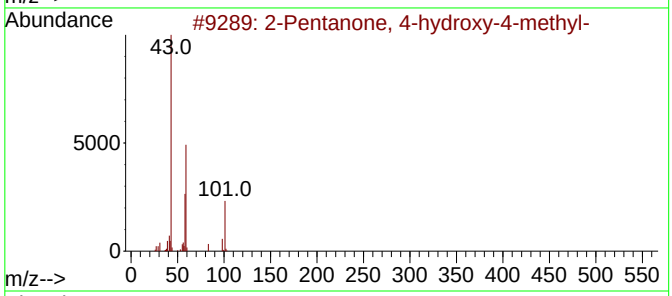
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

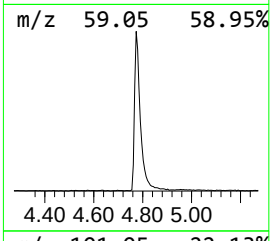
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.773	5.50 ng	83791	1,4-Dichlorobenzene-d4	7.558

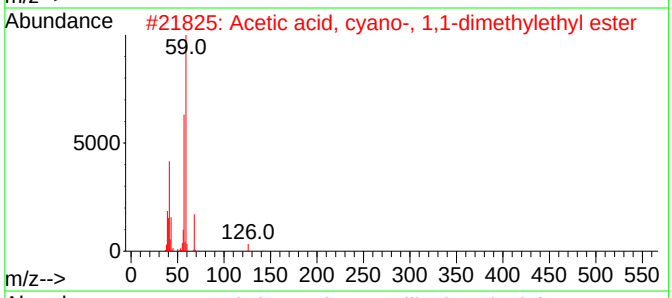
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9

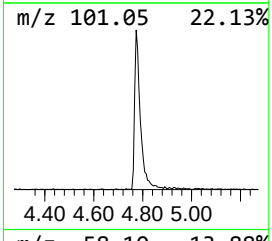


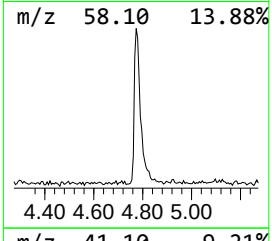


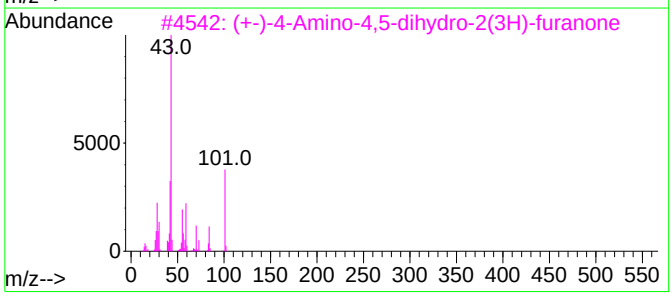


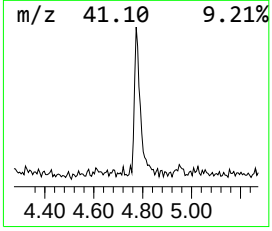












Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE111224\
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Misc :
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Instrument :
BNA_E
ClientSampleId :
LAW-23-00189

Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

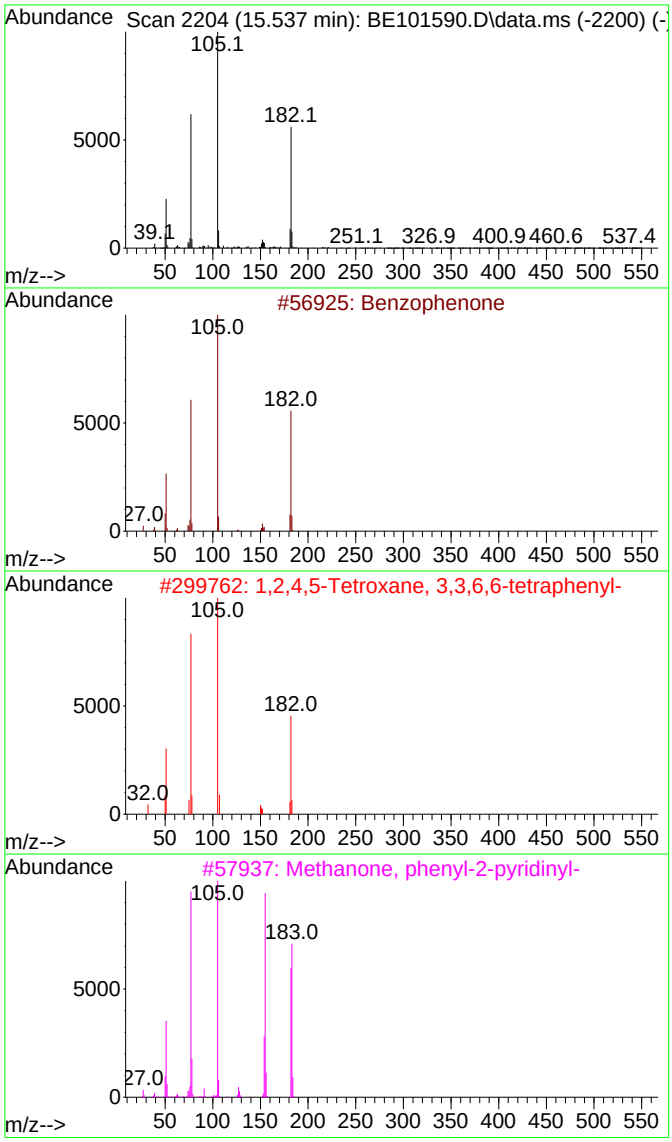
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

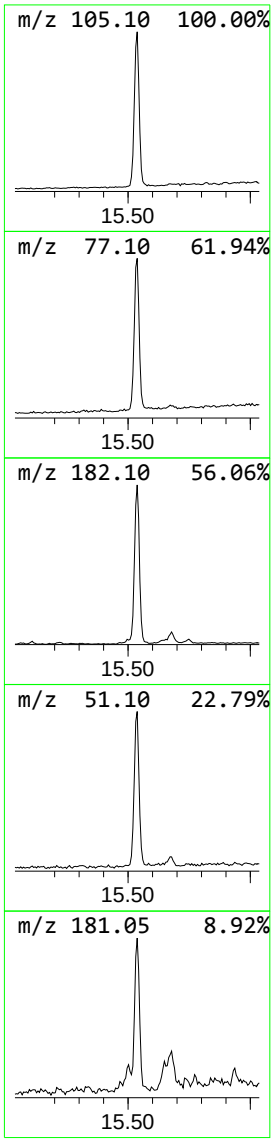
****

Peak Number 5 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.537	4.63 ng	155066	Acenaphthene-d10	14.168

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	64
3	Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	50
4	Benzenamine, N-(3-pyridinylmethy...	182	C12H10N2	029722-97-2	45
5	1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	40





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
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TIC Library : C:\Database\NIST20.L
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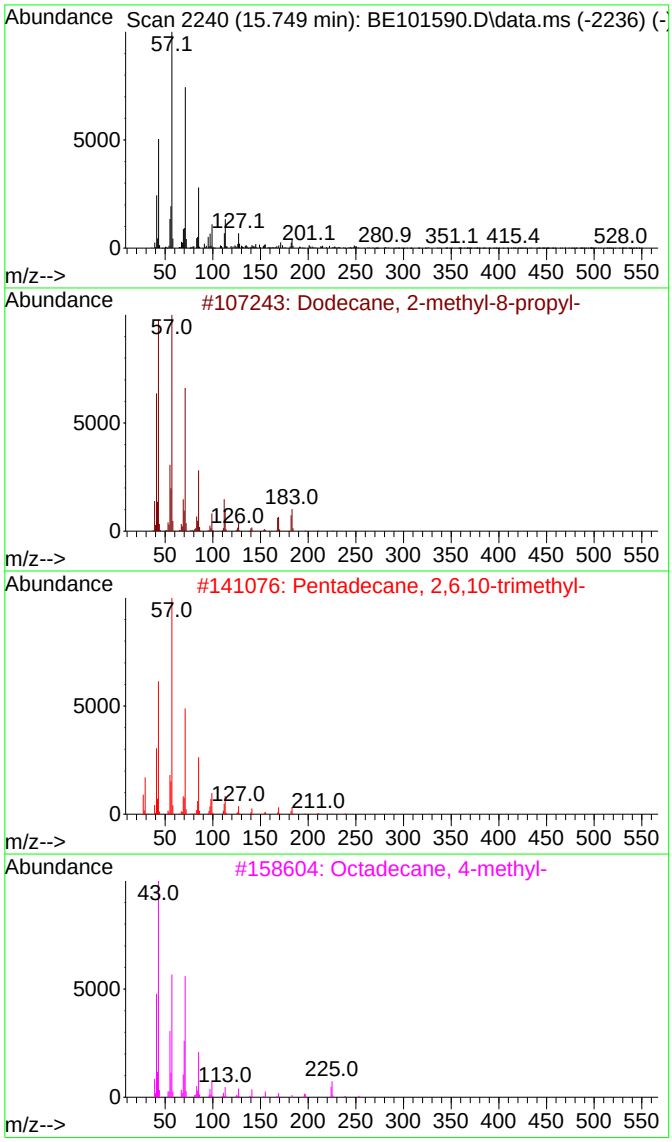
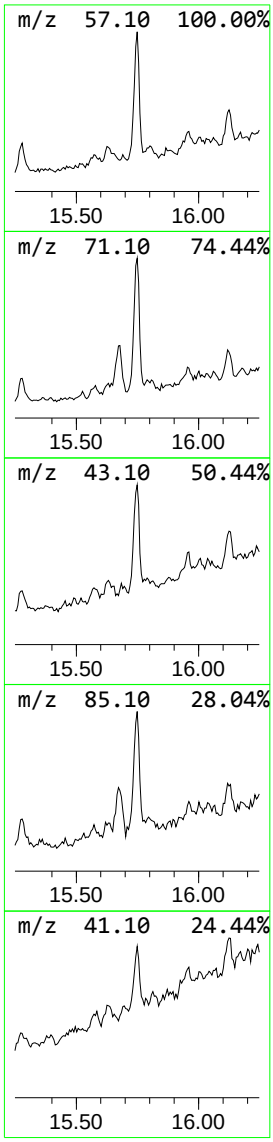
Peak Number 6 Dodecane, 2-methyl-8-propyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.749	3.75 ng	121061	Phenanthrene-d10	16.906

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-8-propyl-	226	C16H34	055045-07-3	91
2	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	87
3	Octadecane, 4-methyl-	268	C19H40	010544-95-3	86
4	Undecane, 6-ethyl-	184	C13H28	017312-60-6	83
5	Pentadecane, 4-methyl-	226	C16H34	002801-87-8	81





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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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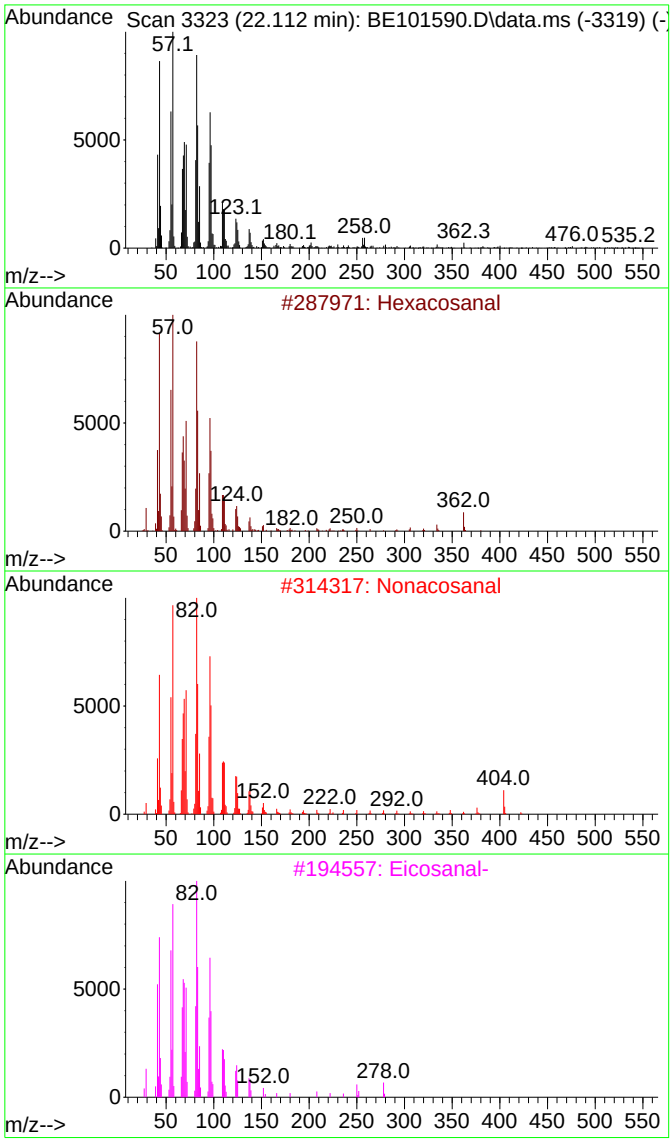
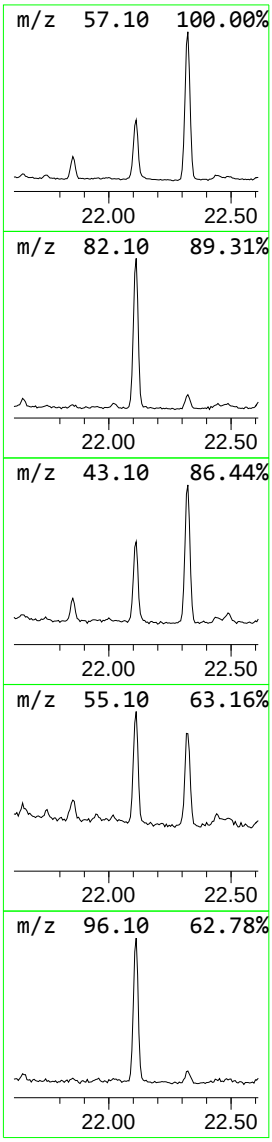
Peak Number 7 Hexacosanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.112	16.48 ng	616582	Chrysene-d12	21.072

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosanal	380	C26H52O	026627-85-0	95
2	Nonacosanal	422	C29H58O	072934-04-4	93
3	Eicosanal-	296	C20H40O	002400-66-0	93
4	Octadecanal	268	C18H36O	000638-66-4	91
5	1,19-Eicosadiene	278	C20H38	014811-95-1	91





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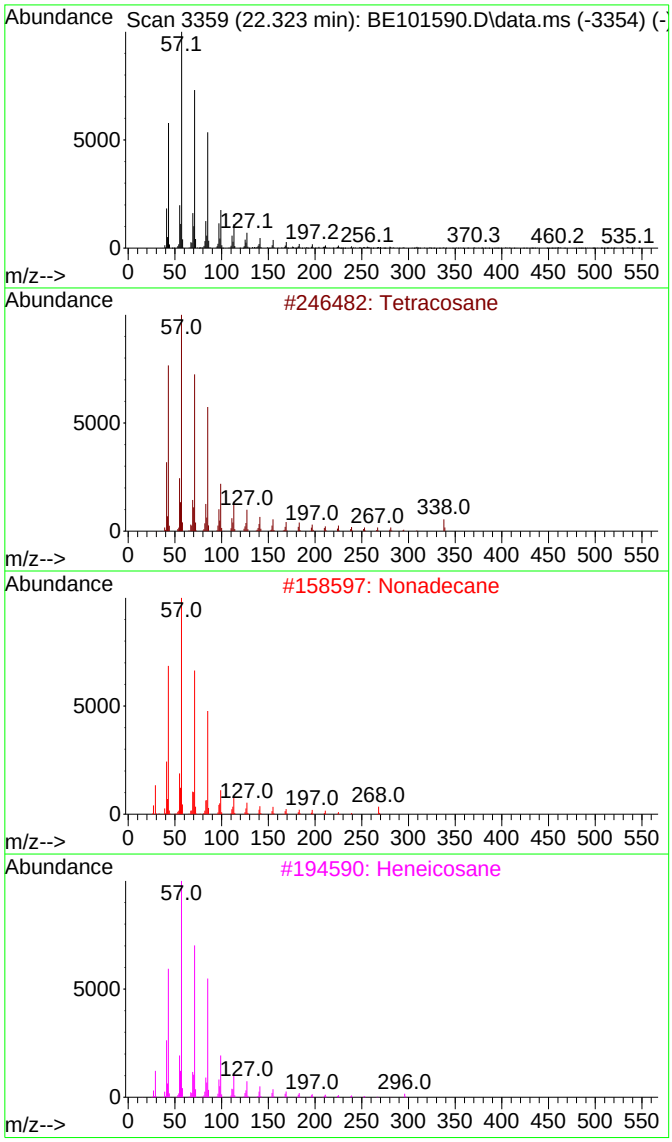
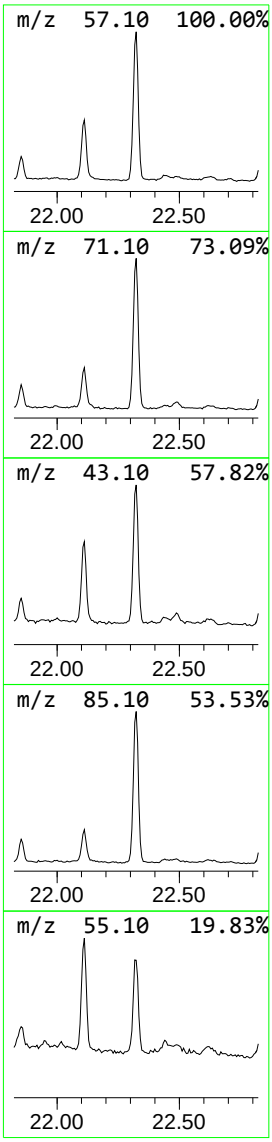
Peak Number 8 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.323	13.04 ng	662873	Perylene-d12	23.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	97
2	Nonadecane	268	C19H40	000629-92-5	94
3	Heneicosane	296	C21H44	000629-94-7	90
4	Nonacosane	408	C29H60	000630-03-5	90
5	Triacontane, 1-iodo-	548	C30H61I	1000406-32-3	90





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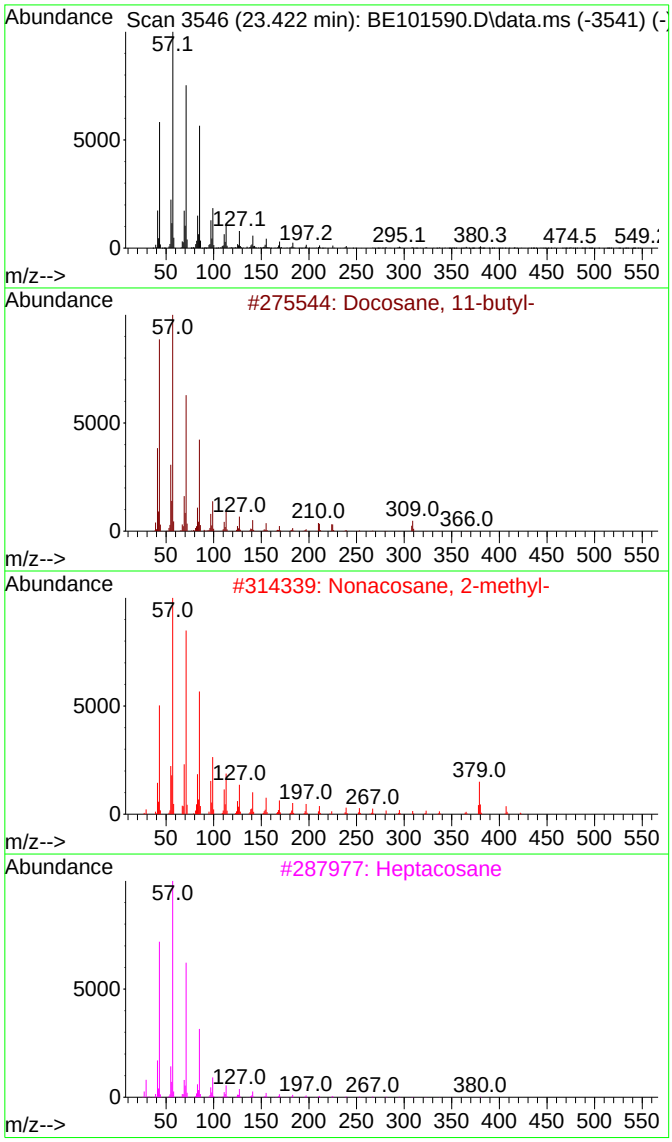
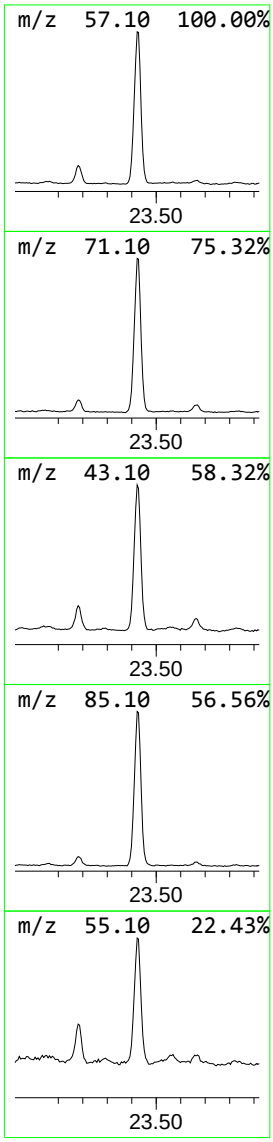
Peak Number 9 Docosane, 11-butyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.422	26.64 ng	1354210	Perylene-d12	23.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 11-butyl-	366	C26H54	013475-76-8	95
2	Nonacosane, 2-methyl-	422	C30H62	001560-75-4	94
3	Heptacosane	380	C27H56	000593-49-7	94
4	Heptadecane	240	C17H36	000629-78-7	93
5	Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE111224\
Data File : BE101590.D
Acq On : 12 Nov 2024 23:58
Operator : RC/JU
Sample : P4795-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
LAW-23-00189

Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

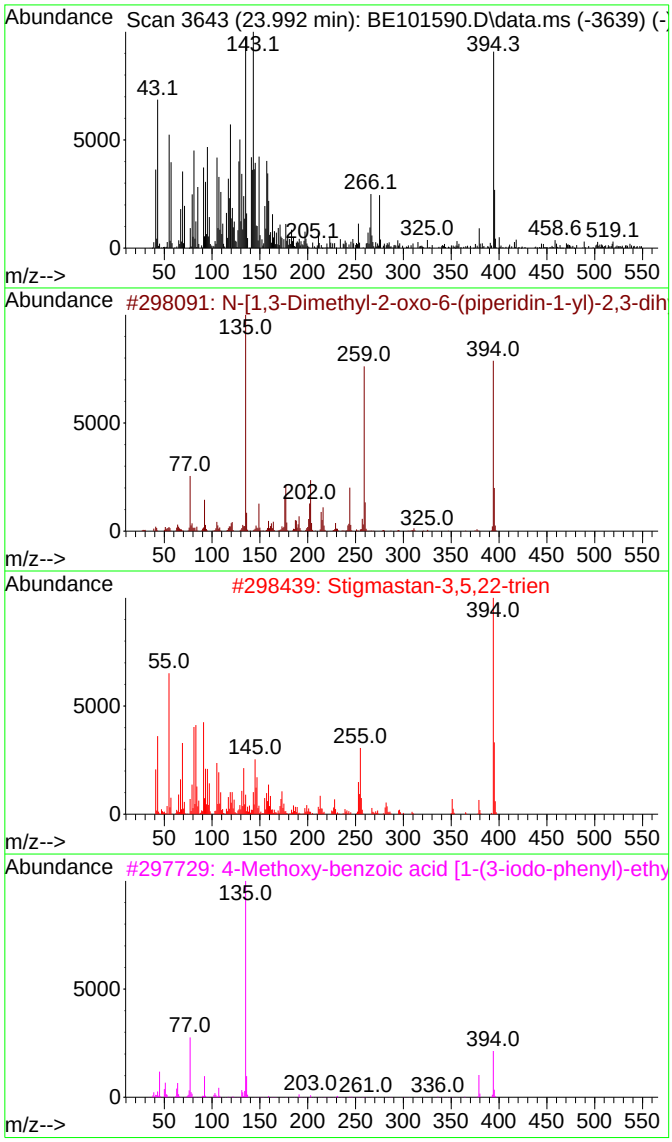
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

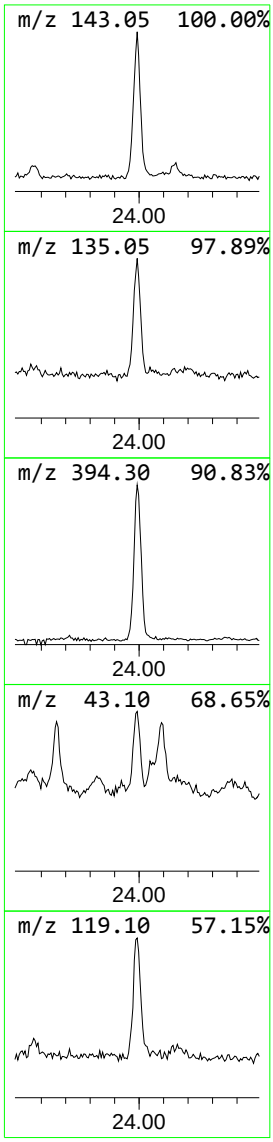
****

Peak Number 10 unknown23.992 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.992	6.15 ng	312654	Perylene-d12	23.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-[1,3-Dimethyl-2-oxo-6-(piperid...	394	C22H26N4O3	901245-65-6	27
2	Stigmastan-3,5,22-trien	394	C29H46	1000214-18-1	18
3	4-Methoxy-benzoic acid [1-(3-iod...	394	C16H15IN2O2	292869-32-0	16
4	Brucine	394	C23H26N2O4	000357-57-3	15
5	3-(3',4'-Dimethoxyphenyl)-7-hydr...	394	C19H13F3O6	1000449-06-3	15





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE111224\
Data File : BE101590.D
Acq On : 12 Nov 2024 23:58
Operator : RC/JU
Sample : P4795-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
LAW-23-00189

Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
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
Propane, 2,2-di...	2.676	82.2	ng	1253140	1	7.558	304831	20.0
Butane, 2-metho...	2.864	23.2	ng	353822	1	7.558	304831	20.0
2-Pentanone, 4-...	4.773	5.5	ng	83791	1	7.558	304831	20.0
Benzophenone	15.537	4.6	ng	155066	3	14.168	669902	20.0
Dodecane, 2-met...	15.749	3.8	ng	121061	4	16.906	646008	20.0
Hexacosanal	22.112	16.5	ng	616582	5	21.072	748108	20.0
Tetracosane	22.323	13.0	ng	662873	6	23.357	1016760	20.0
Docosane, 11-bu...	23.422	26.6	ng	1354210	6	23.357	1016760	20.0
unknown23.992	23.992	6.2	ng	312654	6	23.357	1016760	20.0