LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061221\
Data File : BM030427.D
Acq On : 12 Jun 2021 22:36
Operator : CG/JU
Sample : M2625-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 18-B12(154-158)

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-BM060921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM030427.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.963	314	319	331	rBV	288153	431539	7.12%	0.729%
2	5.416	390	396	407	rBV	1936286	2750619	45.40%	4.644%
3	6.993	657	664	679	rBV	1749877	2828010	46.68%	4.775%
4	7.834	798	807	814	rBV	1313848	2055084	33.92%	3.470%
5	8.987	995	1003	1012	rBV	1111559	1857554	30.66%	3.136%
6	10.416	1234	1246	1264	rBV2	54305	156643	2.59%	0.264%
7	10.622	1273	1281	1291	rBV	1627389	2744604	45.30%	4.634%
8	13.081	1692	1699	1712	rBV	2638702	3976613	65.63%	6.714%
9	13.239	1721	1726	1732	rBV	343909	495587	8.18%	0.837%
10	13.775	1813	1817	1822	rVB	91919	132388	2.19%	0.224%
11	14.063	1859	1866	1872	rVB3	131331	261022	4.31%	0.441%
12	14.228	1888	1894	1897	rBV	128346	202120	3.34%	0.341%
13	14.257	1897	1899	1904	rVB2	69142	92601	1.53%	0.156%
14	14.457	1926	1933	1940	rVV	2452716	3549980	58.59%	5.994%
15	14.522	1940	1944	1956	rVB3	80972	152365	2.51%	0.257%
16	14.775	1983	1987	1989	rBV	63323	85430	1.41%	0.144%
17	14.804	1989	1992	1996	rVB2	82977	106309	1.75%	0.179%
18	15.010	2020	2027	2030	rBV4	149187	275709	4.55%	0.466%
19	15.057	2031	2035	2048	rVB	169988	365834	6.04%	0.618%
20	15.392	2086	2092	2098	rBV	153278	222388	3.67%	0.375%
21	15.939	2179	2185	2193	rVV	1907827	2655009	43.82%	4.483%
22	16.010	2193	2197	2206	rVB2	54605	92563	1.53%	0.156%
23	16.157	2217	2222	2231	rVB4	64296	152319	2.51%	0.257%
24	16.286	2239	2244	2254	rVB6	42066	109740	1.81%	0.185%
25	16.386	2257	2261	2268	rBV3	48060	78802	1.30%	0.133%
26	16.698	2311	2314	2321	rVB3	57797	103529	1.71%	0.175%
27	17.110	2380	2384	2390	rBV6	48135	82479	1.36%	0.139%
28	17.192	2392	2398	2406	rVV	2998769	4178822	68.97%	7.055%
29	17.280	2409	2413	2420	rVB3	61146	99489	1.64%	0.168%
30	18.080	2545	2549	2556	rBV2	155007	236401	3.90%	0.399%
31	19.080	2716	2719	2724	rVB2	106103	131922	2.18%	0.223%
32	19.357	2763	2766	2776	rBV3	84037	132526	2.19%	0.224%
33	19.615	2807	2810	2822	rVB	119257	202863	3.35%	0.343%
34	19.804	2837	2842	2851	rVB	4605487	5476540	90.39%	9.246%
35	20.492	2955	2959	2969	rVB7	126278	287108	4.74%	0.485%
36	20.580	2970	2974	2982	rBV4	140717	355863	5.87%	0.601%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061221\
Data File : BM030427.D
Acq On : 12 Jun 2021 22:36
Operator : CG/JU
Sample : M2625-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 18-B12(154-158)

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-BM060921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.668	2986	2989	2995	rVB3	117693	186675	3.08%	0.315%
38	20.904	3025	3029	3031	rBV	261294	332342	5.49%	0.561%
39	21.068	3053	3057	3063	rBV	209596	304342	5.02%	0.514%
40	21.127	3064	3067	3071	rVB	209665	247927	4.09%	0.419%
41	21.356	3100	3106	3111	rBV	4059813	5318146	87.78%	8.979%
42	21.939	3202	3205	3210	rBV	248314	302351	4.99%	0.510%
43	22.927	3370	3373	3379	rVB	665604	938523	15.49%	1.585%
44	23.633	3487	3493	3507	rVB2	3044573	6058752	100.00%	10.229%
45	24.062	3562	3566	3571	rBV2	435795	792096	13.07%	1.337%
46	24.168	3580	3584	3591	rVB	479750	866905	14.31%	1.464%
47	24.950	3711	3717	3729	rVB4	1669233	4218657	69.63%	7.123%
48	26.421	3961	3967	3986	rVB2	830635	2543267	41.98%	4.294%

Sum of corrected areas: 59228357

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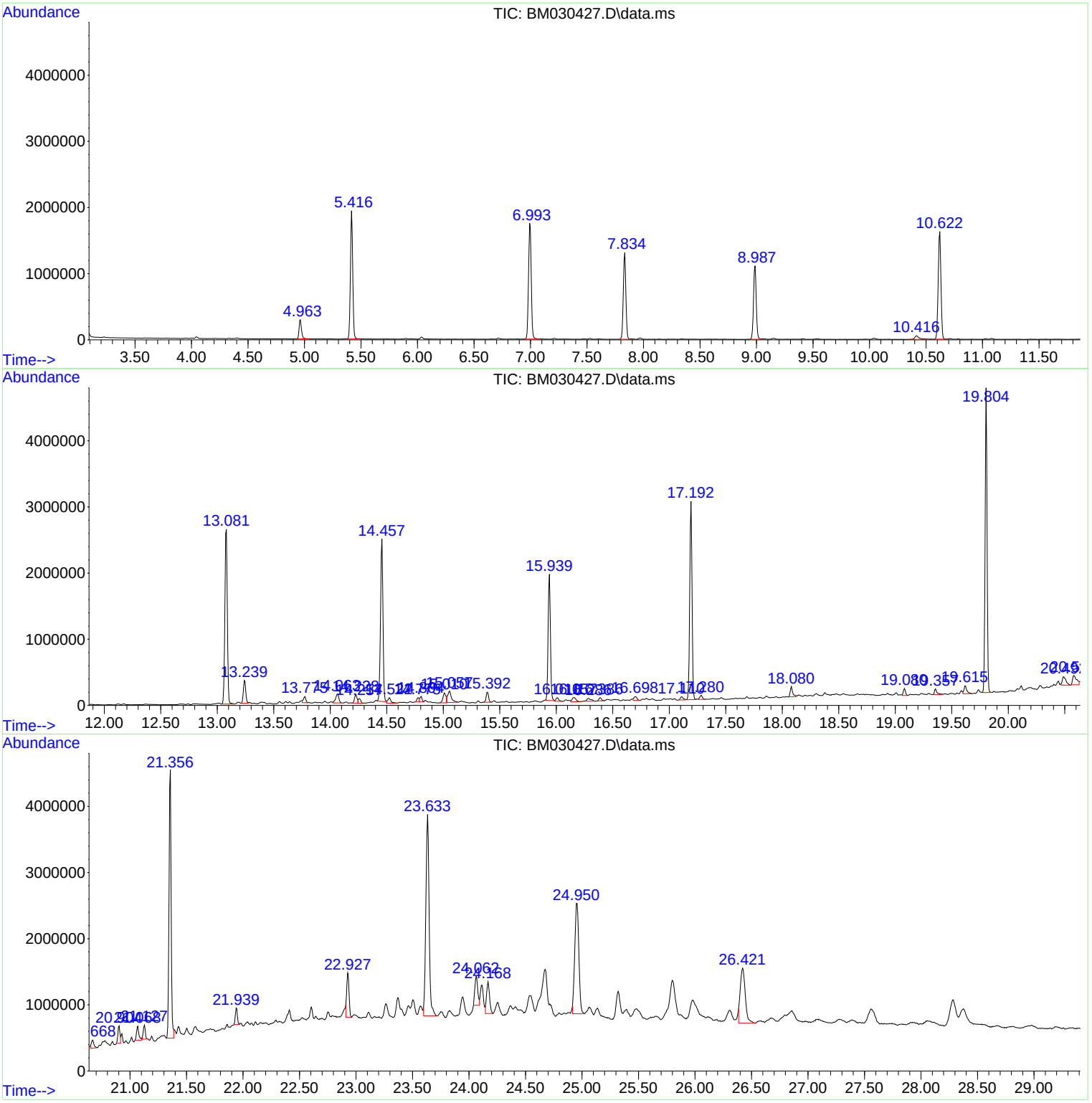
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
18-B12(154-158)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061221\
Data File : BM030427.D
Acq On : 12 Jun 2021 22:36
Operator : CG/JU
Sample : M2625-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
18-B12(154-158)

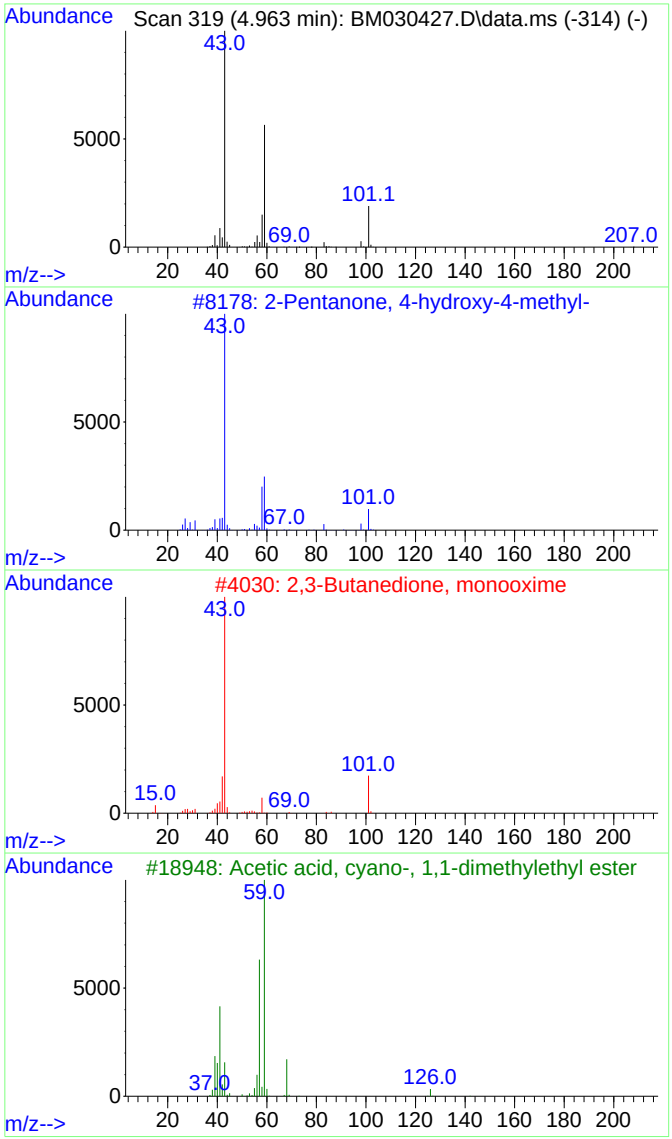
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

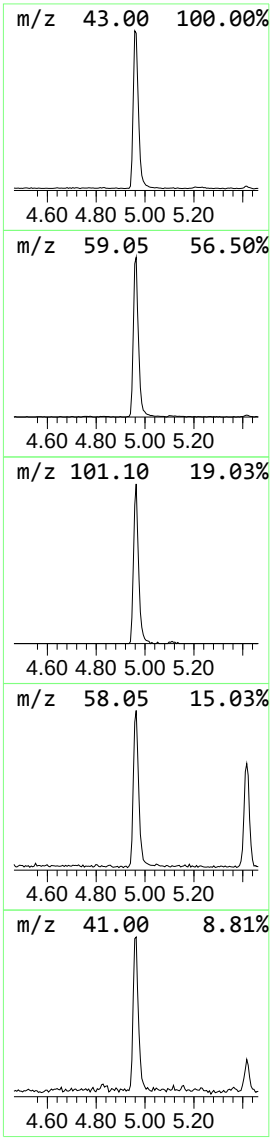
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.963	4.20 ng	431539	1,4-Dichlorobenzene-d4	7.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061221\
Data File : BM030427.D
Acq On : 12 Jun 2021 22:36
Operator : CG/JU
Sample : M2625-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 18-B12(154-158)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

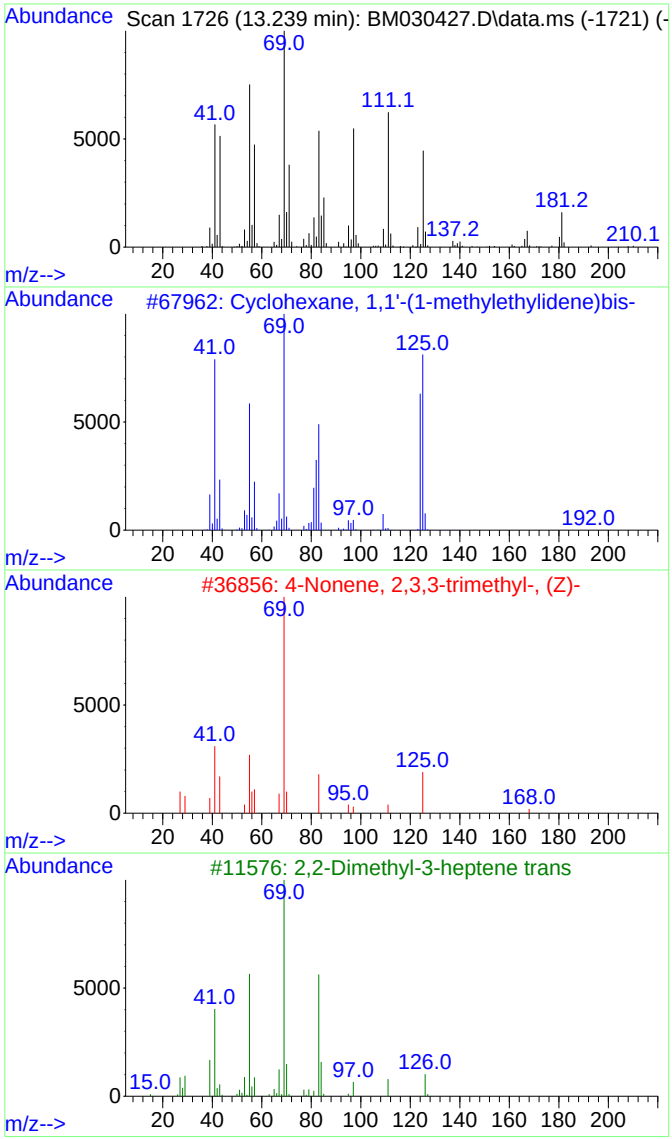
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

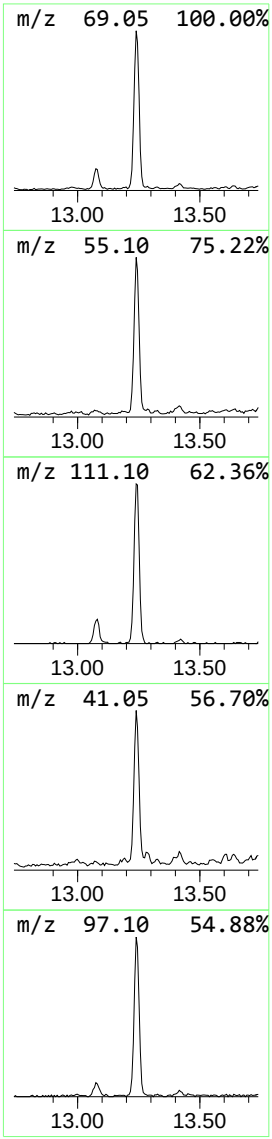
****

Peak Number 2 unknown13.239 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.239	2.79 ng	495587	Acenaphthene-d10	14.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1'-(1-methylethyl...	208	C15H28	054934-90-6	35
2	4-Nonene, 2,3,3-trimethyl-, (Z)-	168	C12H24	063830-68-2	35
3	2,2-Dimethyl-3-heptene trans	126	C9H18	019550-75-5	30
4	Sulfurous acid, cyclohexylmethyl...	304	C16H32O3S	1000309-21-8	30
5	Triallylmethylsilane	166	C10H18Si	001112-91-0	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061221\
Data File : BM030427.D
Acq On : 12 Jun 2021 22:36
Operator : CG/JU
Sample : M2625-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 18-B12(154-158)

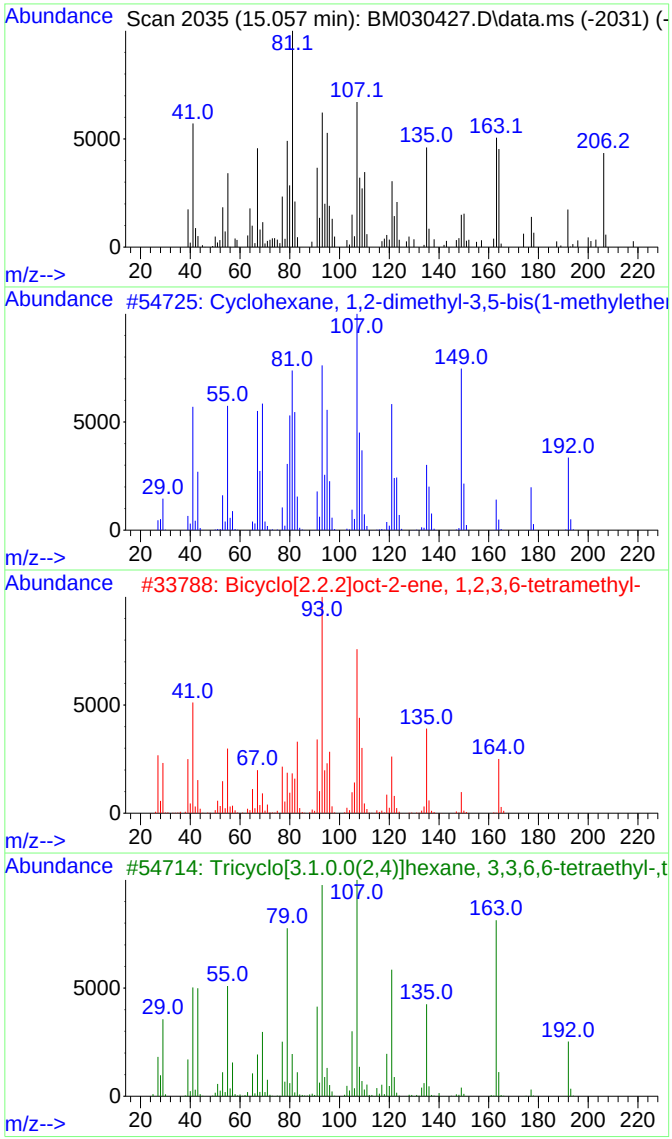
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

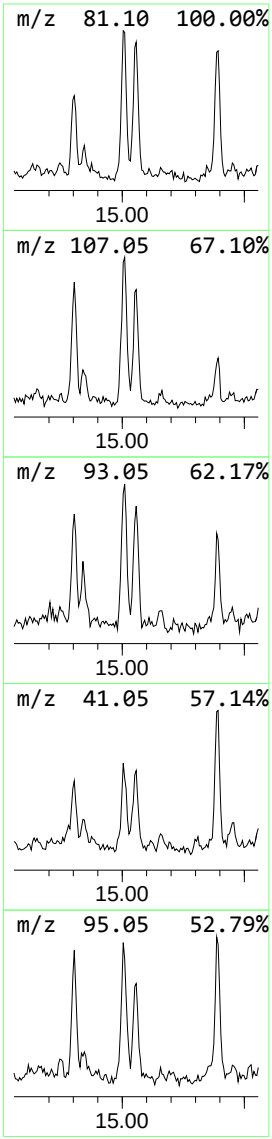
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclohexane, 1,2-dimethyl-3... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.057	2.06 ng	365834	Acenaphthene-d10	14.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2-dimethyl-3,5-bi...	192	C14H24	074806-56-7	64
2	Bicyclo[2.2.2]oct-2-ene, 1,2,3,6...	164	C12H20	062376-14-1	38
3	Tricyclo[3.1.0.0(2,4)]hexane, 3,...	192	C14H24	1000150-14-4	35
4	5-Methyl-2-ethenyl-cyclohexane-1...	168	C10H16O2	1000144-53-6	27
5	Methyl ethyl cyclopentene	110	C8H14	019780-56-4	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061221\
Data File : BM030427.D
Acq On : 12 Jun 2021 22:36
Operator : CG/JU
Sample : M2625-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
18-B12(154-158)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

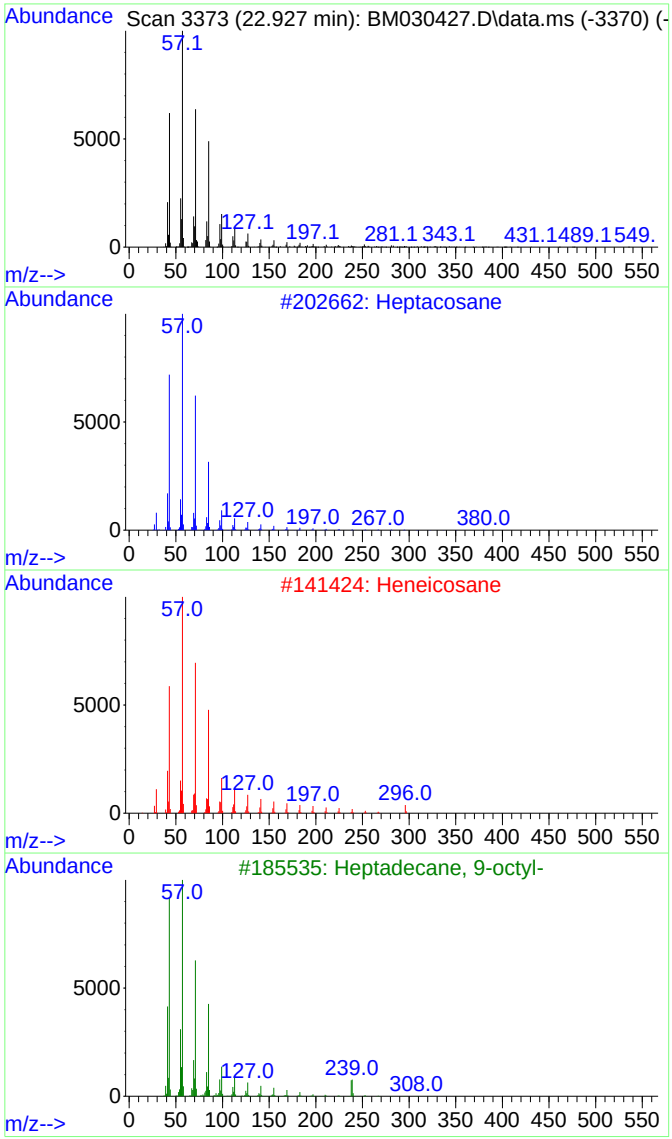
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

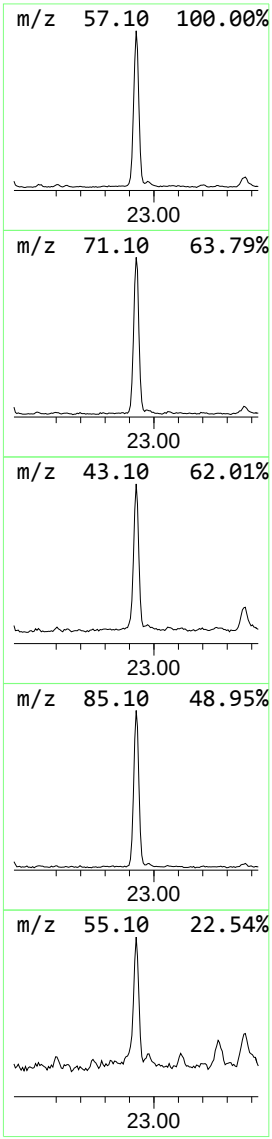
****

Peak Number 4 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.927	3.10 ng	938523	Perylene-d12	23.633

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	95
2	Heneicosane	296	C21H44	000629-94-7	95
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
4	Hexacosane	366	C26H54	000630-01-3	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





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Operator : CG/JU
Sample : M2625-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 18-B12(154-158)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

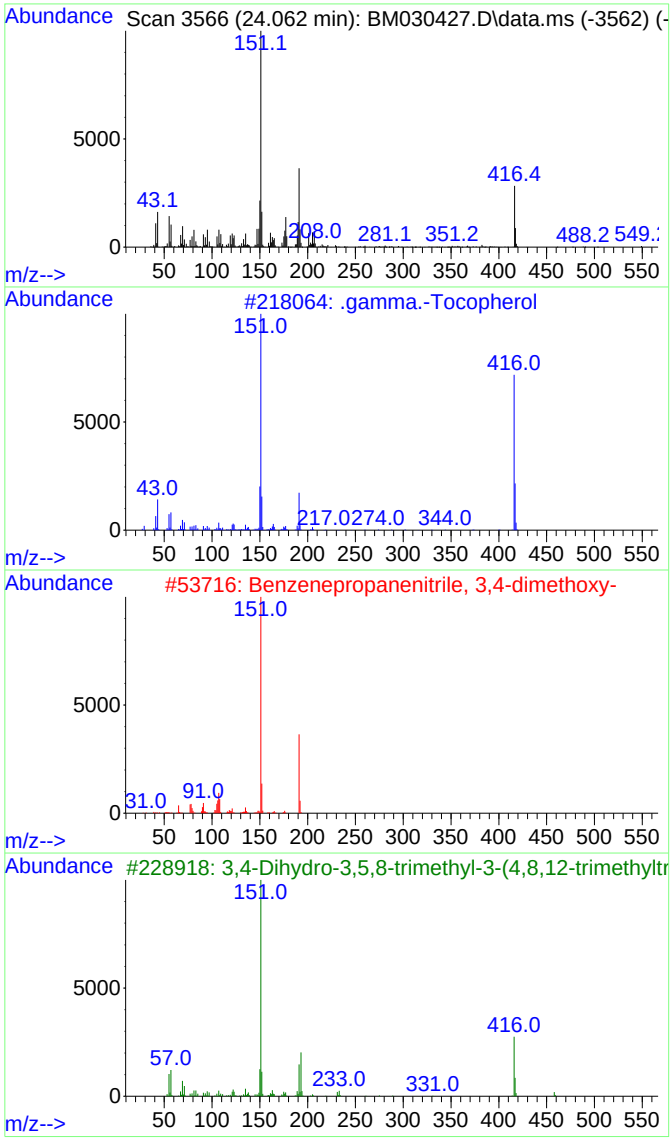
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

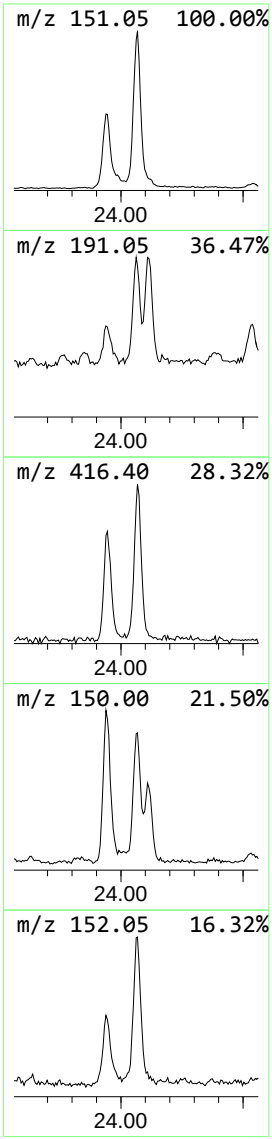
****

Peak Number 5 .gamma.-Tocopherol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.062	2.61 ng	792096	Perylene-d12	23.633

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Tocopherol	416	C28H48O2	007616-22-0	91
2	Benzenepropanenitrile, 3,4-dimet...	191	C11H13NO2	049621-56-9	49
3	3,4-Dihydro-3,5,8-trimethyl-3-(4...	458	C30H50O3	1000105-71-9	45
4	Dimethyl-(allyl)-silyloxybenzene	192	C11H16OSi	066998-68-3	38
5	Ethanone, 2-(1H-imidazo[4,5-b]py...	278	C12H14N4O2S	1000272-55-7	38





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Instrument : BNA_M
ClientSampleId : 18-B12(154-158)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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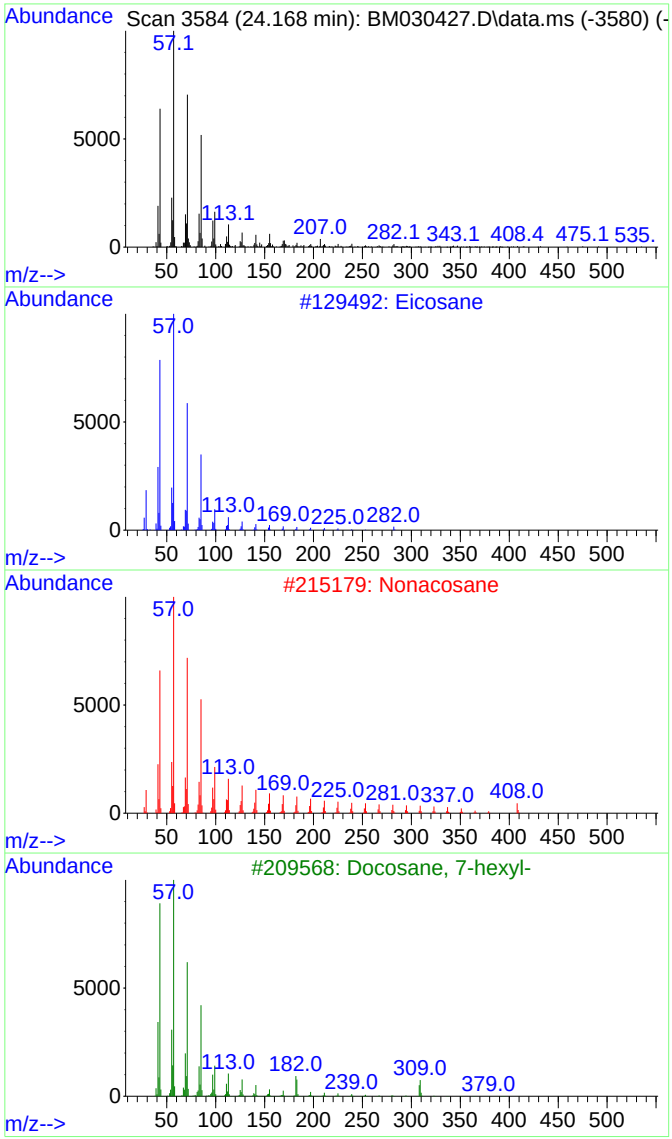
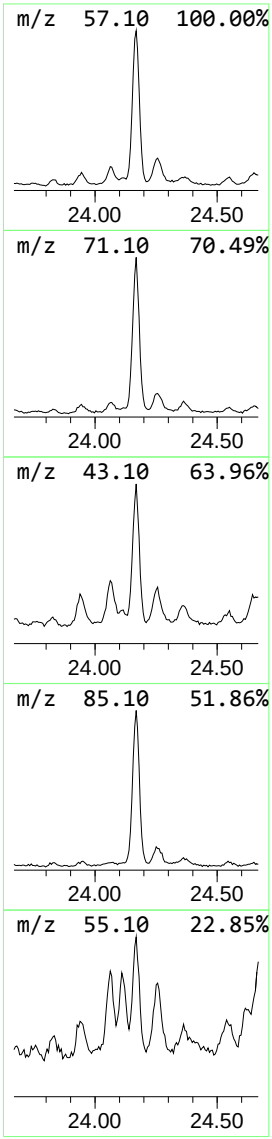
Peak Number 6 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.168	2.86 ng	866905	Perylene-d12	23.633

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Nonacosane	408	C29H60	000630-03-5	95
3	Docosane, 7-hexyl-	394	C28H58	055373-86-9	93
4	Heptadecane, 3-methyl-	254	C18H38	006418-44-6	93
5	Tetracosane	338	C24H50	000646-31-1	90





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Data File : BM030427.D
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BNA_M
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18-B12(154-158)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060921.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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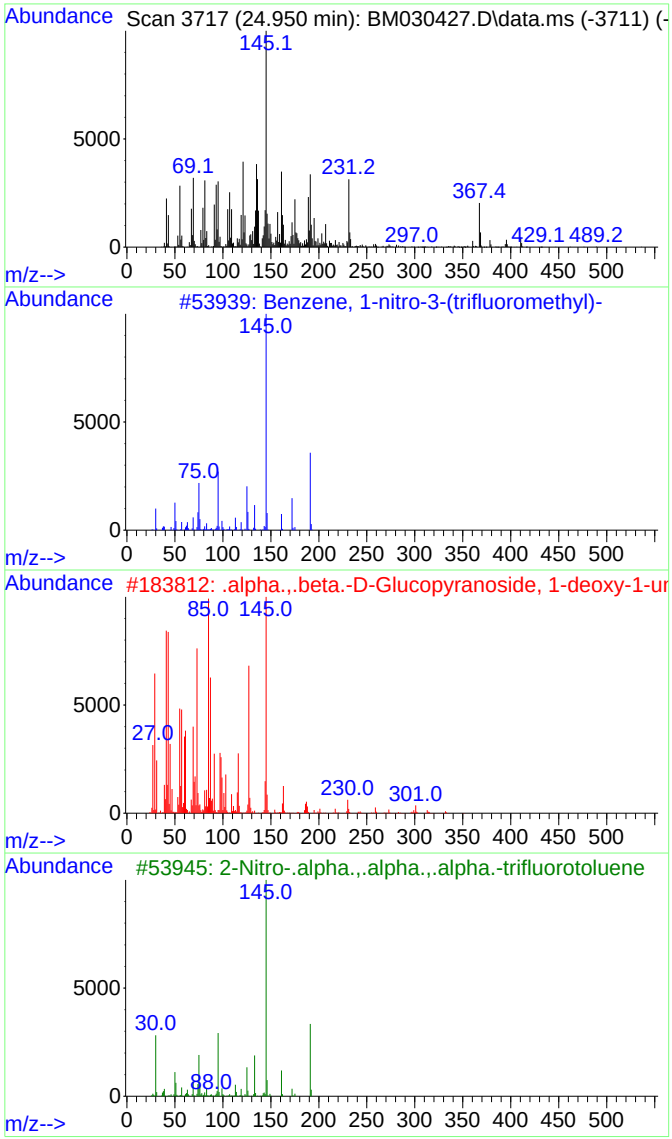
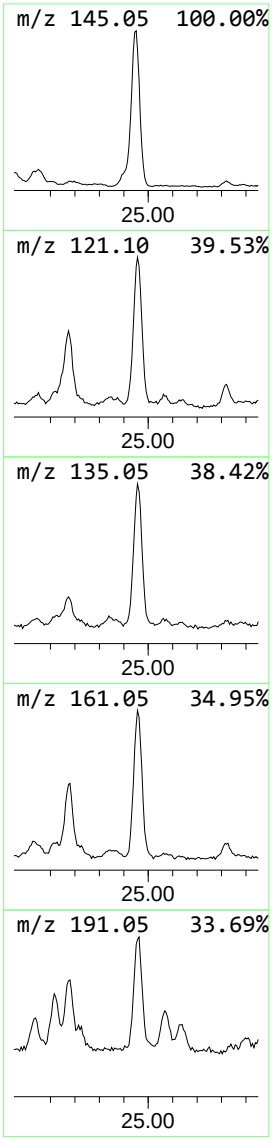
Peak Number 7 unknown24.950 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.950	13.93 ng	4218660	Perylene-d12	23.633

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-nitro-3-(trifluoromet...	191	C7H4F3NO2	000098-46-4	25
2	.alpha.,.beta.-D-Glucopyranoside...	350	C17H34O5S	1000160-71-9	18
3	2-Nitro-.alpha.,.alpha.,.alpha.-...	191	C7H4F3NO2	000384-22-5	17
4	1-Methyl-3-[(N-methylcarbamyloxy...	219	C11H13N3O2	1000212-02-0	16
5	2H-1-Benzopyran, 2,2-dimethyl-	160	C11H12O	002513-25-9	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061221\
Data File : BM030427.D
Acq On : 12 Jun 2021 22:36
Operator : CG/JU
Sample : M2625-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 18-B12(154-158)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

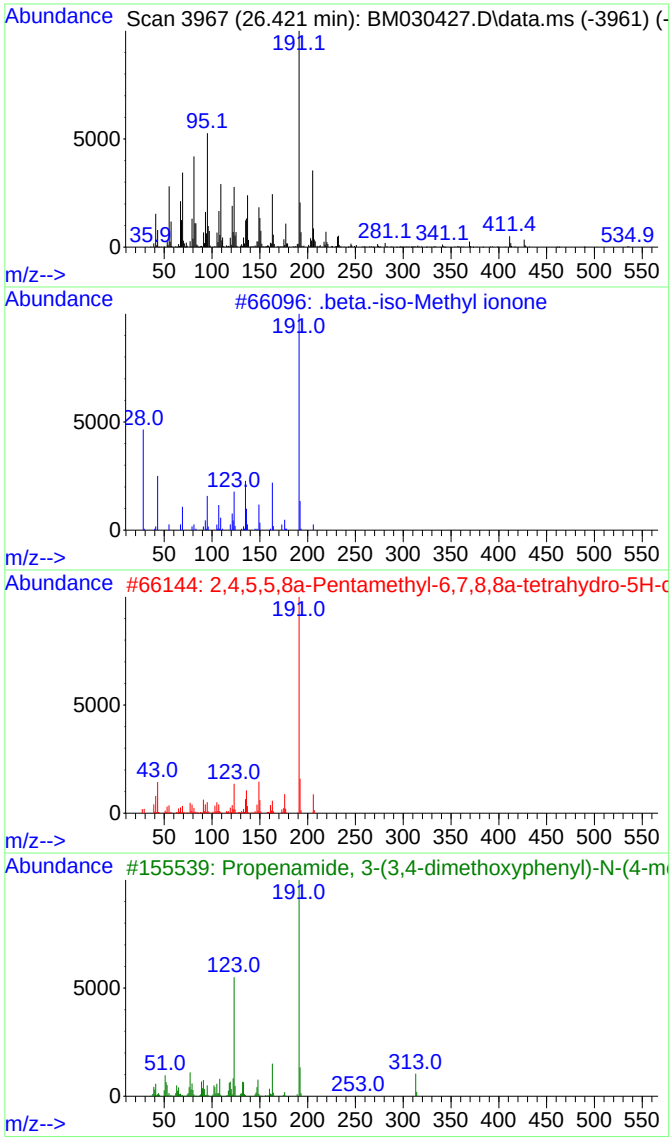
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

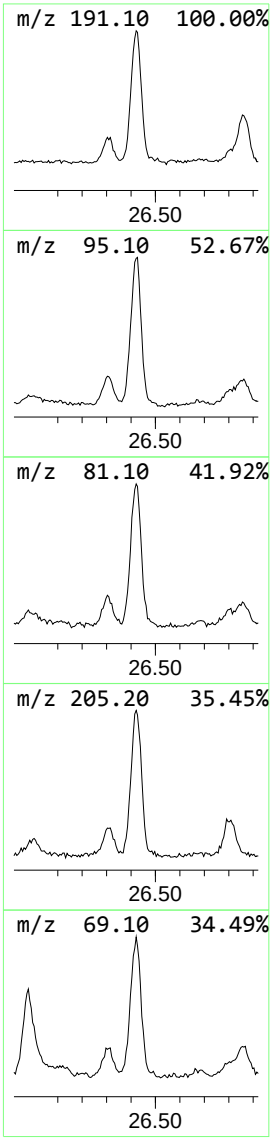
****

Peak Number 8 unknown26.421 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.421	8.40 ng	2543270	Perylene-d12	23.633

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	43
2	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	35
3	Propenamide, 3-(3,4-dimethoxyphe...	313	C18H19NO4	339165-72-9	35
4	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	35
5	4,5-Dihydrothiazol-4-one, 2-(2-m...	222	C10H10N2O2S	022476-61-5	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061221\
Data File : BM030427.D
Acq On : 12 Jun 2021 22:36
Operator : CG/JU
Sample : M2625-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 18-B12(154-158)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060921.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
2-Pentanone, 4-...	4.963	4.2	ng	431539	1	7.834	2055080	20.0
unknown13.239	13.239	2.8	ng	495587	3	14.457	3549980	20.0
Cyclohexane, 1,...	15.057	2.1	ng	365834	3	14.457	3549980	20.0
Heptacosane	22.927	3.1	ng	938523	6	23.633	6058750	20.0
.gamma.-Tocopherol	24.062	2.6	ng	792096	6	23.633	6058750	20.0
Eicosane	24.168	2.9	ng	866905	6	23.633	6058750	20.0
unknown24.950	24.950	13.9	ng	4218660	6	23.633	6058750	20.0
unknown26.421	26.421	8.4	ng	2543270	6	23.633	6058750	20.0